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Lagrangian Operational Dispersion Integrator (LODI) User's Guide

Version 1.0

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Table of Contents

Tables

1. Introduction

The Lagrangian Operational Dispersion Integrator, LODI, is an atmospheric dispersion model developed for operational emergency response within the U.S. Department of Energy's National Atmospheric Release Advisory Center (NARAC). It solves the 3-D advection diffusion equation using a Lagrangian stochastic, Monte Carlo method which calculates possible trajectories of fluid "particles" in a turbulent flow. Particles are marked at the source of a contaminant with an appropriate amount of contaminant mass based upon prescribed mass emission rates. These computational particles can also be given total density and diameters, sampled from an input aerosol size distribution, which are used to calculate gravitational settling and deposition. Initial particle positions are assigned by sampling the spatial distribution based on the geometry of the source. A large number of independent particle trajectories are calculated by moving particles in response to the various processes, such as mean wind advection, gravitational settling and turbulent dispersion, represented within the simulation. The mean contaminant air concentration is estimated from the spatial distribution of the particles at a particular time.

Two key processes are advection by the mean wind and dispersion by turbulent motions. To calculate the mean wind advection, 3-D gridded mean wind fields from the ADAPT model are used as input to LODI. These wind fields may have been derived from observational meteorological data or from another meteorological model. Turbulent dispersion is modeled via a random walk method that uses atmospheric eddy diffusivity (*K*) values to parameterize the effects of turbulent motions that are unresolved by the gridded mean winds. Radioactive decay and production, first-order chemical reactions, bio-agent decay, wet deposition and dry deposition can be simulated.

LODI uses a coordinate system with a continuous terrain representation at the lower boundary. The model supports nested grids and variable grid resolution in both the horizontal and vertical directions. LODI contains several source models including point, line, area, and volume source geometries and buoyancy/momentum driven sources. It can model both instantaneous and continuous sources. Source characteristics such as emission rates, location, and geometry can vary in time. Mean air concentration, time-integrated air concentration, peak mean air concentration, ground deposition, and time-integrated ground exposure (needed for "ground shine" radioactive dose estimates) can be output from LODI.

The features of this model are described in greater detail in the rest of this document which serves as both a model description and a "how to" guide for using the model. Other publications provide further documentation of the development, testing and evaluation of the LODI model (Leone et al., 1997, Nasstrom et al., 2000; Ermak and Nasstrom, 2000; Foster et al., 2000; Larson and Nasstrom, 2002; Sugiyama, et al., 2002; and other publications cited in these).

2. Coordinate Systems

This section describes the different coordinate systems used by LODI. The first spatial coordinate system used is the mapped physical coordinate system, (*x, y, z*), described by any conformal map projection supported by the NARAC system as well as the null projection. In these systems, typically *x* is positive toward the east, *y* is positive toward the north, and *z* is positive "upward". The units are meters.

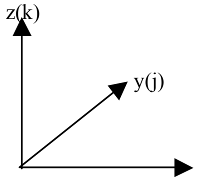

Figure 1. Physical and logical corodinate systems.

In addition to the physical coordinate system, there is a logical coordinate system used in describing the grid structures. This system is the (*i, j, k*) system wherein *i, j*, and *k* are integers which count the grid points in each direction: *i* increasing in the *x* direction, *j* increasing in the *y* direction, and *k* increasing in the *z* direction.

A third coordinate system used by LODI is a transformed physical system, (x', y', σ_z), defined by $x' = x$, $y' = y$, and $\sigma_z = \dfrac{z - z_g(x,y)}{z_T - z_g(x,y)}$ with $z_g(x,y)$ the height of the bottom surface (in *m* above mean sea level, MSL) as a function of *x* and *y*, and z_T the constant altitude of the top of the domain. σ_z values range from 0 at the surface to 1 at z_T, the top of the domain. For convenience this system will usually be denoted as (x, y, σ_z).

The time coordinate system is simply seconds from the problem start time. Within a simulation there are a number of different times specified. The most basic of these is the problem start time and the problem stop times, which determine the simulation time period. A set of meteorological data times specify when meteorological data is available.

In addition, each source has an associated start and stop time that determines the period over which that particular source may emit a contaminant, a set of emission rate times that specify when the emission rate changes, and a set of geometry times, which specify the times when new source geometry information is available.

There are a number of time intervals that control the output of information. First there is the time interval that specifies the frequency of output dumps to the master particle information file and the master deposition file. There is a separate output interval for saving particle position data (which is a whole number divisor of the master particle file output interval). For each concentration field requested there is a time interval that specifies the sampling (and output) interval and a time interval that specifies the length of the sampling for time integrated or averaged samples.

3. Grids

LODI is a Lagrangian model where computational particles are moved through space without respect to a grid. However, grids are needed to 1) define the domain, especially the bottom surface, 2) provide the grid points of the gridded meteorological data, and 3) define the sampling volumes needed to calculate concentrations using the particles. LODI works with two types of grids: meteorological data grids ("met grids" for short) and concentration grids. The purpose of the met grids is to define the domain and the surface topography and to specify the locations of the gridded meteorological data being input to LODI. The concentration grid defines the sampling volumes used to calculate the various output concentration fields.

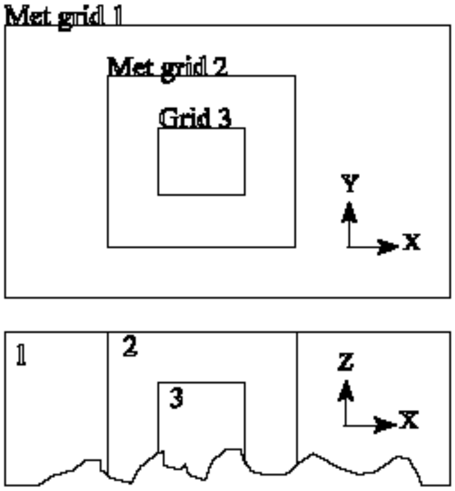

Figure 2. Example of nested meteorological grids in the horizontal (top) and vertical (bottom) planes

To facilitate locating particles within a grid, LODI assumes that all grids, whether met grids or concentration grids, can be described by the Cartesian product of three vectors. For example, to construct a grid that contains 41 nodes in the *x* direction, 51 nodes in the *y* direction, and 19 nodes in the *z* (σ_z) direction, one must define a vector of 41 *x* positions, a vector of 51 *y* positions, and a vector of 19 σ_z positions which increase monotonically. The position of the *i,j,k* node is then simply (x_i, y_j, σ_k). Thus grids with graded or even random spacings in any direction are accepted.

Currently, LODI will accept up to three nested met grids of different resolutions and areas (Figure 2). The first and largest met grid defines the problem domain. Each successive met grid is assumed to be totally contained (nested) within the previous grid. Each met grid is assumed to have a terrain description consistent with its grid resolution. However, the terrain at common nodes along a grid boundary must be the same on each of the grids sharing that node point.

The concentration grid must be fully contained within the outermost met grid and its terrain representation should be consistent with that of the met grids. (This will happen automatically if the concentration grid is made via the NARAC GRIDGEN software.) The concentration grid will often be graded in each horizontal direction with the grid spacing increasing away from the source location and in the vertical with grid spacing increasing with height above ground. This allows higher resolution sampling of the concentrations near the source. However, the user can define the sampling grid in any way that would seem to fit the problem best. For example an elevated source with a corresponding elevated sampling bin may call for the finest vertical spacing near the release height.

4. Meteorological Data

There are currently two ways that LODI receives meteorological data. Three-dimensional gridded data is read from standard NARAC met data formatted netCDF files. This data may be on up to three nested grids, with each grid having its own data files. Data that is not spatially varying within the model is specified via namelist file input.

To handle the time dependence of the meteorological data, the user must list a set of meteorological data times which specify the valid times of the data. LODI will linearly interpolate the meteorological data in time to calculate the value at the current time. If only one meteorological data time is specified, LODI will assume that the meteorological data is constant in time. For times before the first met time, the first met data set values are used. For times after the last meteorological data time, LODI assumes persistence and uses the last meteorological data set values.

The wind field components, $\overline{u}, \overline{v}, \overline{w}\,((\bar{x}, \bar{y}, \bar{z}))$, where ($x, y, z$) are the projection coordinates (i.e., the supplied wind field is the wind on the grid projection), the vertical turbulent diffusivity, K_z, the horizontal velocity variance, σ_v^2, the turbulence time scale, T_i, the friction velocity, u_*, the inverse Monin-Obukhov length, L^{-1}, and the boundary layer height at the grid points are read from the metdata files in netCDF format. There must be one netCDF data file for each meteorological time and for each nested meteorological grid. Thus, if a simulation uses 15 meteorological data times and two meteorological data grids, 30 meteorological data netCDF files are required.

For model testing versus analytic solutions or cases when external turbulence data is not available, it is possible to read just the wind field from the netCDF files and then specify turbulence parameters via namelist input. Each variable must be assigned a list of values with one value that applies throughout the simulation domain for each meteorological data time. When the turbulence data is being set via the namelist, the friction velocity, u_*, may be input via the namelist or may be calculated as a spatially varying field by the model based upon a user input surface roughness length, z_0, and the wind fields.

5. Basic Equation

To model dispersion within the atmosphere, LODI solves the three-dimensional, incompressible, advection-diffusion equation with sources and sinks:

$$\frac{\partial\overline{C}}{\partial t} = -\overline{u}\frac{\partial\overline{C}}{\partial x} - \overline{v}\frac{\partial\overline{C}}{\partial y} - \overline{w}\frac{\partial\overline{C}}{\partial z} + \frac{\partial}{\partial x}\left(K_x\frac{\partial\overline{C}}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y\frac{\partial\overline{C}}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_z\frac{\partial\overline{C}}{\partial z}\right) + w_s\frac{\partial\overline{C}}{\partial z} - \Lambda\overline{C} - \lambda\overline{C} + Q, \qquad \textbf{(1)}$$

where $\overline{C}$ is the mean air concentration of the species; $\overline{u}$, $\overline{v}$, and $\overline{w}$ are the mean wind components in the *x, y*, and *z* projection directions respectively; *t* is time; K_x, K_y, and K_z are the eddy diffusivities for the three coordinate directions (the eddy diffusivity tensor is assumed to be diagonal); w_s is the absolute value of the gravitational settling velocity; Λ is the precipitation scavenging coefficient; λ is the decay (or rate) constant; and *Q* is the source term.

LODI solves the stochastic differential equations that describe the same process as equation (4) within a Lagrangian framework (Durbin, 1983). The equations for the particle displacement due to advection, diffusion, and settling in the three coordinate directions are:

$$dx = \overline{u}dt + (2K_x)^{1/2}dW_x, \qquad \textbf{(2)}$$

$$dy = \overline{v}dt + (2K_y)^{1/2}dW_y, \qquad \textbf{(3)}$$

$$dz = \overline{w}dt + \frac{\partial K_z}{\partial z}dt + (2K_z)^{1/2}dW_z - w_s dt \qquad \textbf{(4)}$$

where $dW_{x,y,z}$ are three independent random variates with zero mean and variance *dt*. (It has been assumed that turbulence is approximately homogeneous in the horizontal, *x* and *y*, directions, i.e., $\partial K_x/\partial x$ and $\partial K_y/\partial y$ are negligible). The stochastic differential equations above are then integrated in time to calculate an independent trajectory for each particle. The ensemble-mean concentration, at any time *t,* can then be calculated from the particle locations at time *t* and the contaminant mass associated with each particle.

6. Numerical Methods

The integration method used to calculate the particle trajectories is a two-step process. First, a random displacement due to turbulent diffusion is calculated using either (1) a Gaussian particle position probability density function or (2) the skewed, non-Gaussian particle position probability density function developed and successfully tested by Ermak and Nasstrom (2000). For the Gaussian function, the new particle position z_{i+1} at time t_{i+1} is generated, given the initial position z_i at t_i, from a Gaussian probability density function with mean and variance given by

$$\overline{z} = z_i + v_i\Delta t \qquad \textbf{(5)}$$

$$\sigma_{z\,D}^2 \equiv \overline{(z_{i+1} - \overline{z})^2} = 2K_{zi}\Delta t + v_i^2\Delta t^2 \qquad \textbf{(6)}$$

where $\Delta t = t_{i+1} - t_i$, $K_{zi} \equiv K_z(z_i)$, and $v_i \equiv \left(\partial K_z/\partial z\right)_{z=z_i}$. For the skewed, non-Gaussian probability density function, the third central moment, given by

$$\varsigma_z^3 \equiv \overline{\left(z_{i+1} - \bar{z}\right)^3} = 6K_{zi}v_i\Delta t^2 + 2v_i^3\Delta t^3, \qquad \textbf{(7)}$$

is used in addition to the mean and variance to define the function. Ermak and Nasstrom showed that the non-Gaussian function can be significantly more efficient than the commonly used Gaussian function for cases where the eddy diffusivity varies linearly with height to zero at a boundary, as in the surface layer similarity theory relationships given in Section 7.2.3. The displacement due to turbulent diffusion in the *z* direction during Δt is then $\Delta z_{i,turb} = z_{i+1} - z_i$. Similar equations are used for the *x* and *y* directions. However, since the spatial derivatives of the eddy diffusivity in these directions are assumed to be negligible, a Gaussian function is always used for random displacements in the *x* and *y* directions. The available options for characterizing the horizontal and vertical eddy diffusivities, *K_x*, *K_y*, and *K_z*, are described in Section 7.

Next the mean wind velocities are used to calculate the final particle position using a second order Runge-Kutta method:

$$\Delta x_i = \frac{1}{2}(k1_{xi} + k2_{xi}), \qquad \textbf{(8)}$$

$$\Delta y_i = \frac{1}{2}\left(k1_{yi} + k2_{yi}\right), \qquad \textbf{(9)}$$

$$\Delta z_i = \frac{1}{2}\left(k1_{zi} + k2_{zi}\right), \qquad \textbf{(10)}$$

where $$k1_{xi} = \bar{u}\left(x_i, y_i, z_i, t_i\right)\Delta t_i + \Delta x_{i,turb},$$

and $$k2_{xi} = \bar{u}\left(x_i + k1_{xi}, y_i + k1_{yi}, z_i + k1_{zi}, t_i + \Delta t_i\right)\Delta t_i + \Delta x_{i,turb}$$

and similarly for the *y* and *z* directions, (In the *z* direction the mean velocity used may include settling and plume rise, in addition to the mean wind velocity.)

To maintain accuracy and maximize efficiency, the model uses an adaptive time step, which is calculated for each particle at each step. To resolve spatial variations in the met fields, each particle is restricted to a time step that allows it to move on average no more than one grid cell, unless this is overridden by user input. If particles move below ground due to turbulent diffusion or mean wind advection, they are, by default, reflected above ground (see “reflect” parameter in “prob_setup” namelist).

7. Internal Turbulence Parameterizations

7.1 Introduction

This section describes turbulence parameterizations used in LODI, which provide eddy diffusivity, *K*, values for diffusion calculation in cases where turbulence data is not read from the meteorological data files.

Several parameterization options are available in order to (a) provide options for applications in the atmosphere and (b) provide options useful in testing versus analytic solutions. The turbulence parameterization options for the *vertical* direction are described in Subsection 2. This is followed in Subsection 3 by a discussion of those for the *horizontal* directions.

7.2 Vertical turbulence parameterizations

7.2.1 Constant K_z

K_z can be fixed at a user-input constant value applied throughout the grid. When used with a constant wind velocity, this option allows calculations to be compared to a Gaussian analytic solution of the advection-diffusion equation.

7.2.2 Linear-Power Law K_z

Another option that is useful for testing against known solutions is the power law form defined by:

$$K_z(z) = \begin{cases} \left.\dfrac{dK_z}{dz}\right|_{z=z_g} (z - z_g)\left(1 - \dfrac{z - z_g}{H}\right)^n & \text{for } 0 \le z - z_g \le H, \\ 0 & \text{for } z - z_g > H \end{cases} \qquad \textbf{(11)}$$

where n, and H are constants specified by the user. Note that this option can be used to obtain a linear equation for K_z as a function of z by specifying H to be greater than or equal to the top of the grid and $n = 0$ in the power law reducing equation (11) to,

$$K_z(z) = \left.\frac{dK_z}{dz}\right|_{z=z_g} (z - z_g), \quad (z - z_g) \ge 0. \qquad \textbf{(12)}$$

7.2.3 Similarity theory K_z

Similarity theory can be used to specify K_z profiles as functions of the surface and boundary layer scaling parameters u_* , the friction velocity, h, the boundary layer height, z-z_g, the height above ground, and L, the Monin-Obukhov length. Within the boundary layer (z-$z_g < h$),

$$K_z^{bl}(z) = \frac{ku_*(z - z_g)}{\varphi_h} e^{-\frac{c(z-z_g)}{h}} \qquad \textbf{(13)}$$

(Lange, 1989) where

$$\varphi_h = \left(1 + a\frac{z - z_g}{L}\right)^b, \qquad \textbf{(14)}$$

$$a = \begin{cases} -16 \text{ if } \dfrac{1}{L} < 0 \\ 0 \text{ if } \dfrac{1}{L} = 0, \\ 5 \text{ if } \dfrac{1}{L} > 0 \end{cases} \quad b = \begin{cases} -\dfrac{1}{2}, \text{ if } \dfrac{1}{L} < 0 \\ 1, \text{ if } \dfrac{1}{L} \ge 0 \end{cases}, \quad c = 4. \text{ and } k = 0.4$$

For the free troposphere *(z-$z_g > h$)*, K_z is constant with height with a default value of

$$K_z^{tropo} = 0.01\frac{m^2}{s},$$

The default values given above for K_z^{tropo} and c can optionally be overridden by user input. Values for *1/L* and h must be input by the user while u_* may be input by the user via a namelist variable or it may be calculated as a horizontally varying array in the code.

7.3 Horizontal turbulence parameterizations

7.3.1 Constant K_H

This option allows $K_x = K_y$ to be fixed at a user-input constant value, K_H, unchanging with height or downwind distance. When used with a constant wind velocity, this constant K_H option allows validation versus analytic solutions to the 3-D diffusion equation.

7.3.2 Horizontal eddy diffusivity from velocity variance and time scale

The assumptions implicit in the advection-diffusion equation are not valid at travel times shorter than the Lagrangian velocity correlation time. However, horizontal velocity fluctuations often exhibit long correlation times. To compensate for this, travel-time-dependent horizontal eddy diffusivities are used, with K_x and K_y determined from semi-empirical relationships based on statistical dispersion theory for stationary, homogeneous turbulence. The following relationship between the time-dependent variance of the cross-wind concentration distribution, σ_y^2, and the eddy diffusivity is used:

$$K_y = \frac{1}{2}\frac{d\sigma_y^2}{dt}. \qquad \textbf{(15)}$$

and (Draxler, 1976):

$$\sigma_y = \frac{\sigma_v t_a}{1 + D\left(\frac{t_a}{T_i}\right)^{1/2}}, \qquad \textbf{(16)}$$

where $D = 0.9$, σ_v is the standard deviation of the cross-wind velocity component, t_a is the time since the material was released at a point source, and T_i is an empirical time scale which is related to the Lagrangian correlation time of the cross-wind velocity component. It is assumed that $K_x = K_y$.

Using the previous two equations, the following equation for K_y can be derived:

$$K_y = \sigma_v^2 t_a \frac{1 + \frac{D}{2}\left(\frac{t_a}{T_i}\right)^{1/2}}{\left[1 + D\left(\frac{t_a}{T_i}\right)^{1/2}\right]^3} \qquad \textbf{(17)}$$

The variation of K_y with time t_a over a computational time step may be significant, especially since as $t_a \rightarrow 0$, $K_y \rightarrow 0$. Therefore, for a given computational time step from $t = t_i$ to $t_i + \Delta t_i$ the value of K_{yi} used for a particle for that time step is calculated as follows:

$$K_{yi} = K_y\Big|_{t_a = t_i - t_0} + \tfrac{1}{2}\Delta t_i \frac{\partial K_y}{\partial t_a}\Big|_{t_a = t_i - t_0}, \qquad \textbf{(18)}$$

(t_0 is the time the particle was emitted from the source) where

$$\frac{\partial K_y}{\partial t_a} = \sigma_v^2 \frac{\left[1 + \frac{D}{4}\left(\frac{t_a}{T_i}\right)^{\frac{1}{2}}\right]}{\left[1 + D\left(\frac{t_a}{T_i}\right)^{\frac{1}{2}}\right]^4}. \qquad \textbf{(19)}$$

The local value of the velocity variance and time scale at the particle position can be used to determine the horizontal diffusivities at any given time in the calculation, assuming that the turbulence can be locally approximated as homogeneous and stationary.

For cases where external turbulence data is not available in the meteorological data files, there are two options for determining values of σ_v and T_i. In the first option (turb_param_h = 'sigmav'), the user may input time-varying (but spatially constant) values of σ_v and T_i via the namelist. The second and preferred option (turb_param_h = 'sigmav_simthry') is calculates space- and time-varying values of σ_v and T_i as a function of *z*, *u**, *L,* and *h* as discussed below. This option allows the calculated values of σ_v to be scaled using a time-varying measured value input via the namelist.

The following similarity scaling relationship for the variance of the horizontal velocity components is used in the unstable ABL ($1/L < 0, z - z_g < h$):

$$\sigma_v^2 = Au_*^2\left(1 - \frac{z - z_g}{h}\right)^{\frac{3}{2}} + Bw_*^2 \qquad \textbf{(20)}$$

where $A = 4.25$, $B = 0.34$, and ($z - z_g$) is the height above ground level. The form of this relationship was proposed by Rodean (1996). It accounts for both shear-generated turbulence through the term with friction velocity, u_*, and buoyancy-generated turbulence (through the term with convective velocity scale, w_*). (Note that $w_*^3 / u_*^3 = -h/kL$). In the surface layer, it is similar to the relationship used by Panofsky *et al.* (1977). In the convective limit (large $-h/L$ and w_* / u_*), it is consistent with observations of σ_u^2 and σ_v^2 that are approximately constant with height in the convective boundary layer (Caughey and Palmer, 1979). For slightly unstable conditions, it is consistent with the decreasing variance with height found by Nicholls and Readings (1979).

The following relationship is used in stable and neutral ABL $\left(L^{-1} \geq 0,\ z - z_g < h\right)$:

$$\sigma_v^2 = Au_*^2\left(1 - \frac{z - z_g}{h}\right)^{\frac{3}{2}} \qquad \textbf{(21)}$$

and is based on the relationships determined by Nieuwstadt (1985) and Lenschow *et al.* (1988). For consistency between the stable and unstable relationships in the neutral limit, the value $A = 4.25$ is used. It is intermediate between the Panofsky *et al.* value of 4.0 for the neutral and unstable surface layer and the Lenschow *et al.* value of 4.5 at the surface for the stable surface layer. The crosswind and along-wind velocity component variances are assumed to be equal, $\sigma_v^2 = \sigma_u^2$.

The idealized conditions (e.g., stationary, horizontally-homogeneous) assumed by similarity theory scaling relationships are not always found in the atmospheric boundary layer (ABL). In the stable boundary layer, the turbulent properties may depend primarily on local fluxes, rather than surface fluxes, and turbulence may be intermittent under very stable conditions. In addition, other processes (e.g., topographically and thermally forced motions, clouds, and gravity waves) which are not accounted for in these scaling relationships may have a significant effect on velocity variances. For these reasons, measured values of velocity variances are always preferred. Values are most often measured near the surface. If a measured value, $\sigma_{v\,m}^2(z_m)$, is available at a measurement height, z_m, then the parameterized variance values at all heights are scaled to match the measurement, i.e.,

$$\sigma_{v\,ps}^2(z) = \frac{\sigma_{v_m}^2(z_m)}{\sigma_{v\,p}^2(z_m)}\sigma_{v\,p}^2(z) \quad \textbf{(22)}$$

where $\sigma_v^2(z)$ is the parameterized value calculated at height z using the relationships given above and $\sigma_{v\,ps}^2(z)$ is the scaled value used in the model calculation. Irwin and Paumier (1990) found that this approach resulted in reasonable agreement between scaled parameterized turbulence values and observed values throughout the depth of the convective boundary layer.

For low-wind-speed, stable conditions, several investigators (Hanna, 1983; Leahy *et al.*, 1988; Etling, 1990; Hanna and Chang, 1992) have found that observations of horizontal velocity variances near the surface tend to approach constant values for averaging periods of one hour, and do not continue to decrease with decreasing wind speed and friction velocity, as indicated by the above parameterizations. Hour-average minimum values for σ_v found by these investigators range from 0.2 to 1.0 m s^{-1} for low wind speed, stable conditions at a variety of sites. Therefore, a minimum velocity variance value is used for all heights and stability conditions, i.e.,

$$\sigma_v^2(z) = \max\left\{\sigma_{v\,ps}^2(z), \sigma_{v\,\min}^2\right\} \quad \textbf{(23)}$$

where $\sigma_{v\,ps}^2(z)$ is the parameterized value calculated at height z, and $\sigma_{v\,\min}^2$ is a specified minimum value. The default value of $\sigma_{v_{\min}} = 0.5\ \mathrm{m\,s^{-1}}$ $\left(\sigma_{v\,\min}^2 = 0.25\right)$ may be overridden by user input.

Velocity variance depends on averaging time. For averaging periods of less than one hour, velocity variance values may be smaller than the minimum value assumed for one hour period. If representative observations with averaging periods less than one hour are available, they can be input and used in the model to scale the parameterized values, as discussed above.

Considerably less is known about scaling turbulence properties above the boundary layer, than within the boundary layer. The very limited number of observations of $\sigma_u$and σ_v in the stable layer above the entrainment layer presented by Caughey and Palmer (1979) and above the near-neutral boundary layer presented by Brost *et al.* (1982) are in the range of 0.2 to 0.8 m s^{-1}. Therefore, above the boundary layer, $z \geq h$, the constant value $\sigma_v^2 = 0.25$ is used.

For the neutral and stable ABL ($1/L \geq 0, z < h$), the value T_i = 1000 s proposed by Draxler (1976) is used. This value is also used for $z > h$ for all stability conditions. For the unstable ABL ($1/L < 0$, $z < h$),

$$T_i = \frac{h}{\left(27u_*^3 + 1.2w_*^3\right)^{1/3}}$$

based on the σ_y relationship developed by Briggs (1985) for the convective boundary layer (large $-h/L$ and w_*/u_*) and the approach developed by Nieuwstadt and van Duuren (1978) for interpolating between the neutral limit ($w_* = 0$) and convective limit ($w_* >> u_*$). Briggs used a mathematical form for σ_y that is somewhat different from Draxler's. In order to use the same mathematical form for both stable and unstable conditions, the relationship for T_i was determined so that Draxler's form for σ_y, used in this model, closely fit Briggs' σ_y relationship in the convective limit. The value T_i can be overridden by user input in the namelist.

8. Settling and Deposition

8.1 Settling velocity

The terminal settling velocity, w_s, is based on the particle diameter, particle density, air density, and air viscosity using methods described by Hinds (1982). The method used depends on the Reynolds number of the flow around the falling particle. For a spherical particle of diameter d_p falling at terminal settling velocity w_s relative to the air, the Reynolds number is

$$\mathrm{Re} = \frac{\rho w_s d_p}{\mu} \quad \textbf{(24)}$$

where ρ is the air density, and μ is the dynamic viscosity of the air. For small Reynolds number, Stokes law is valid and is used to calculate the terminal settling velocity:

$$w_s = \frac{\rho_p d_p^2 g}{18\mu}, \quad \text{for } Re < 1 \quad \textbf{(25)}$$

where ρ_p is the particle density, and g is the gravitational acceleration.

We do not use the Cunningham correction factor (a multiplicative factor applied to the Stokes law settling velocity) for small particles (d_p < 1 μm at standard temperature and pressure) and low air pressure. For atmospheric dispersion problems, this correction factor does not have a significant effect because the settling velocities are extremely small compared to vertical motions due to turbulence and the mean wind. For example, for diameters ranging from 0.01 to 1.0 μm, settling velocities are on the order of 10^{-7} to 10^{-5} m/s, for standard temperature and pressure, and the Cunningham correction factor ranges from approximately 22 to 1.2, respectively.

Since Stokes law is not valid for Reynolds number greater than one, we use the following general expression for the settling velocity:

$$w_s = \left(\frac{4\rho_p d_p g}{3C_D\rho}\right)^{1/2}, \quad \text{for } Re > 1 \quad \textbf{(26)}$$

where C_D is the coefficient of drag. However, this expression cannot be used directly to determine w_s because C_D depends on Re which, in turn, depends on w_s. We use the approach, described by Hinds (1982), for computing the quantity $C_D Re^2$,

$$C_D \mathrm{Re}^2 = \frac{4 d_p^3 \rho_p \rho g}{3\mu^2} \quad \textbf{(27)}$$

which does not depend on w_s. Re is then determined by interpolating between tabulated values of Re versus $C_D Re^2$ for settling spheres published by McDonald (1960) and Hinds (1982). The settling velocity is then given by

$$w_s = \frac{\mu \mathrm{Re}}{\rho d_p} \quad \textbf{(28)}$$

Air density and dynamic viscosity values, needed for these calculations, are currently calculated using standard temperature and pressure.

8.2 Deposition velocities

Dry deposition is parameterized in terms of a deposition velocity, $v_d > 0$, at a reference height z_r (typically 1-1.5 m over land surfaces and 10-15 m over ocean surfaces; Sehmel, 1980). The dry deposition flux onto the surface is then given by $v_d C(z_r)$, where $C(z_r)$ is the air concentration at height z_r. The deposition velocity parameterizes the effect of all near-surface dry deposition processes below the reference height including: turbulent and molecular diffusion to the surface, inertial impaction on surface, absorption by the surface, as well as gravitational settling. Therefore, deposition velocities depend on (a) particle diameter, (b) particle density, (c) chemical species, (d) turbulent properties of the surface layer, (e) atmospheric state variables, and (f) surface characteristics (e.g., vegetation).

The deposition velocity is composed of two independent velocities: w_d, the "non-settling deposition velocity", and w_s, the gravitational settling velocity. The non-settling deposition velocity is calculated in terms of a resistance model. The integral resistance (e.g., in units of s/m) to deposition below a reference height is written as the sum of three resistances,

$$r_T = r_a + r_b + r_c \qquad \textbf{(29)}$$

where r_a is the aerodynamic resistance (which is a function of the turbulent properties of the surface layer), r_b is the resistance of the quasi-laminar sub-layer near the surface (which is a function of the molecular diffusivity of the species, among other variables), and r_c is the bulk surface resistance (e.g., Wesely, 1989). One can then define

$$w_d \equiv \frac{1}{r_T} \qquad \textbf{(30)}$$

The deposition velocity for gaseous species ($w_s = 0$) can be expressed as

$$v_d = w_d . \qquad \textbf{(31)}$$

For particulate matter ($w_s > 0$), the deposition velocity is a function of both w_d and w_s, and is given by

$$v_d = \frac{w_s}{1 - e^{-w_s / w_d}} \qquad \textbf{(32)}$$

(Sehmel and Hodgson, 1978).

8.3 Settling and dry deposition

For settling and dry deposition calculations, the vertical model domain is divided into two regions: the pure gravitation settling region and a near surface layer of depth Δz_d, the dry deposition layer (see Figure 3). Within the pure gravitational settling region, the vertical displacement of a particle due to settling is simply:

$$\Delta z_d = -w_s \Delta t. \qquad \textbf{(33)}$$

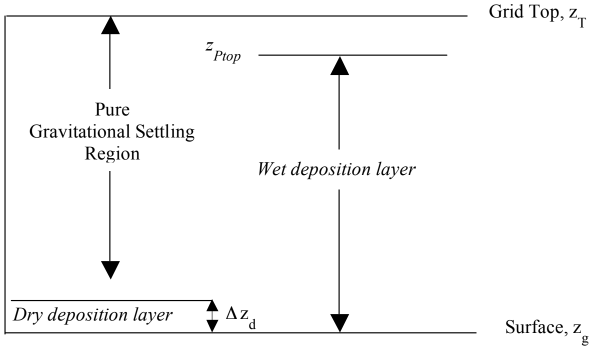

Figure 3: Relationships of deposition layer heights in LODI.

(All settling and deposition velocities are defined to be positive downward by convention.)

Within the dry deposition layer, z < z_g + Δz_d, the dry deposition of material onto the surface is calculated by depleting the mass of the particles and allowing them to exponentially approach the surface. By depleting mass from all particles near the surface, instead of entirely removing whole particles to account for deposition, the statistical signifance of both the deposition and air concentration calculations is dramatically improved (by maintaining a larger particle count for both calculations). During time increment Δt, the particle position is calculated by,

$$z(t+\Delta t) - z_g = \left[z(t) - z_g\right] e^{-\left(\frac{w_s}{\Delta z_d}\right)\Delta t}, \qquad \textbf{(34)}$$

and the mass associated with the particle is depleted (due to dry deposition alone) according to

$$m(t+\Delta t) \;=\; m(t) e^{-\frac{v_d \Delta t}{\Delta z_d}}. \qquad \textbf{(35)}$$

The mass of this particle deposited on the surface due to dry deposition during Δt is then

$$\Delta m_D(\Delta t) = m(t)\left[1 - e^{-\left(\frac{v_d}{\Delta z_d}\right)\Delta t}\right]. \qquad \textbf{(36)}$$

The resulting deposition flux onto the bottom surface is

$$j_d(t) \;=\; \frac{v_d}{\Delta z_d} \int_0^{\Delta z_d} C(z,t)\,dz, \qquad \textbf{(37)}$$

Note that if $C(z) = C_0$ is constant with height in the deposition layer, then $j_d = v_d C_0$.

8.4 Wet deposition

If the precipitation scavenging coefficient, Λ, is greater than zero and the particle is within the wet deposition layer, i.e. its height is below the top of the precipitation layer height, $z_{Ptop}(t)$, at time t , then the mass of a particle is depleted as follows:

$$m(t+\Delta t) = m(t)e^{-\Lambda \Delta t}. \qquad \textbf{(38)}$$

The mass due to wet deposition that is deposited during Δt at the surface (in the grid cell directly below the particle position) is then

$$\Delta m_w(\Delta t) = m(t)\left[1 - e^{-\Lambda \Delta t}\right]. \qquad \textbf{(39)}$$

9. Decay and Reaction Processes

9.1 Radioactive decay

The change in the air or ground concentration of a radionuclide due to radioactive decay and production is simulated using analytic solutions to the coupled first-order ordinary differential equations describing this process based on a method developed by R. Freis (personal communication, 1999). Simultaneous decay and production of radionuclides in radioactive decay chains can be simulated. Radionuclide decay constants and decay branching fractions are obtained from a database developed at Oak Ridge National Laboratory (1980).

Single or multiple radionuclides may be associated with each source. Radionuclides associated with a single source (in the "species" namelist parameter) and any daughter products they produce are assumed to remain together as they are transported and deposited, and, therefore, are associated with the same computational particles. The concentration and deposition of daughter products that are produced from parent radionuclides are calculated by the model, and may be output to concentration files, even if they are not specified in the "species" parameter of the source namelist.

For the simple case of decay without daughter products a simple decay constant, λ, can be input through the "lambda" namelist input parameter for the appropriate source namelist (optionally half life or efolding time can be entered). If $\lambda > 0$, then mass of a particle is depleted during Δt according to

$$a(t + \Delta t) = a(t)e^{-\lambda\Delta t} \quad . \qquad \textbf{(40)}$$

where *a* represents activity associated with a particle.

9.2 Chemical reactions

First-order chemical reactions may be simulated by specifying the rate constant, λ, in the "lambda" namelist input parameter for the appropriate source. Equation (40) is then applied with mass replacing activity.

9.3 Ultra-violet radiation decay of biological agents

The viability of biological agents is often sensitive to UV radiation. In order to simulate this effect, we have implemented a simple decay model that calculates the decay rate (% per minute) due to UV radiation as a function of the midday and night decay rates and the solar angle. The equation used is

$$r_{uv} = r_{uvmin} + (r_{uvmax} - r_{uvmin}) * \sin(\theta) \qquad \textbf{(41)}$$

where r_{uvmin} and r_{uvmax} are the minimum and maximum decay rates respectively in units of % per minute of the agent, and θ is the solar elevation angle. (Note that the information on the decay rates of most biological agents is very limited and typically consists of a decay rate quoted at a single temperature and humidity level.) The solar angle is calculated from the latitude and longitude of the source (assuming this is representative of the particle location), the date, and the time of day.

10. Source Descriptions

A LODI source describes the emission of one or more species from a single location (all species in a source must have the same decay parameters). It is specified by a collection of input parameters giving the location and spatial distribution of the source of the emission, the time period of the emission, the emission rate, the species emitted and their characteristics such as half-life, deposition velocity, aerosol mass size distribution, etc., and the desired number of particles to be used to represent this source. A list of all source parameters is contained in the src_param namelist described in Table 5. In the sections below, the source geometries (i.e., the spatial distribution of mass emitted by the source) supported by LODI are described as well as the conventions used to define the emission rates.

10.1 Source geometries

Five different source geometries are available to specify the distribution of mass (activity): a line source, a truncated Gaussian source with cutoffs and rotation, a point source, a circular area source, and a spherical source. In addition, it is possible to read an existing LODI-compatible netCDF particle file to provide source information.

For simplicity, each of the source geometries is described below for a single time. However, all the geometry parameters can vary in time. Thus, for a given source, a set of geometry valid times are specified and each geometry parameter is specified for each of these times. LODI will then use a linear time interpolation to determine the source at any particular instant.

10.1.1 A line source

Particles are emitted uniformly distributed along a specified line segment in three dimensional space between two points (x_1,y_1,z_1) and (x_2,y_2,z_2) via,

$$\begin{aligned} y(x) &= -\frac{y_2 - y_1}{x_2 - x_1}(x_2 - x) + y_2 \\ z(x) &= -\frac{z_2 - z_1}{x_2 - x_1}(x_2 - x) + z_2 \end{aligned} \qquad \textbf{(42)}$$

for $x_1 \le x \le x_2$.

10.1.2 A Gaussian source

Particle (*x, y, z*) locations are randomly sampled from a truncated Gaussian distribution with a specified mean and standard deviation in each coordinate direction independently,

$$P(x,y,z) = \frac{1}{(2\pi)^{3/2} * std_x * std_y * std_z} e^{-\frac{1}{2}\left[\left(\frac{x-mean_x}{std_x}\right)^2 + \left(\frac{y-mean_y}{std_y}\right)^2 + \left(\frac{z-mean_z}{std_z}\right)^2\right]} \qquad \textbf{(43)}$$

for

$$\begin{cases} (mean_x - cutoff\_dx\_\min) \le x \le (mean_x + cutoff\_dx\_\max) \\ (mean_y - cutoff\_dy\_\min) \le y \le (mean_y + cutoff\_dy\_\max) \\ (mean_z - cutoff\_dz\_\min) \le z \le (mean_z + cutoff\_dz\_\max) \end{cases} \qquad \textbf{(44)}$$

where the cutoffs are user specified.

For sources that are not symmetric about the x and/or y axis the Gaussian source may be rotated in the horizontal plane by a rotation angle, angle_deg, between 0 and 90

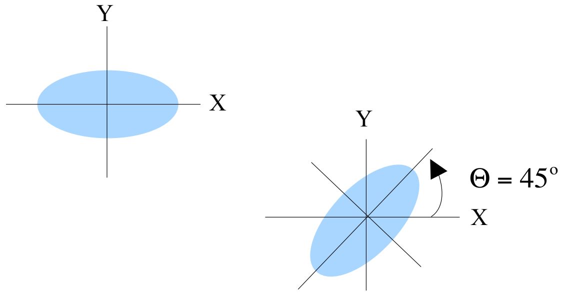

Figure 4. Source rotation by an angle Θ from the x axis.

degrees counter-clockwise from the x axis. Figure 4 illustrates the effect of specifying a rotation of 45^o.

10.1.3 Spherical source

Particle locations are randomly picked from a uniform distribution within a sphere with a user specified center, (x_center, y_center, z_center), and radius.

10.1.4 Point source

Particles are released at a user specified point, (x_pt, y_pt, z_pt).

As an example of a time-dependent source geometry, a moving point source can be described by giving its position at three different times, for example, 0, 100, 500 seconds. The user would specify the three geometry times 0, 100, and 500 seconds, and then the 3 corresponding values of (x_pt, y_pt, z_pt).

10.1.5 Horizontal circular area source

Particle locations are randomly picked from a uniform distribution to cover a horizontal circular area with a user defined center, (x_center, y_center), radius, and height (z_center). This source is usually used in combination with plume rise calculations.

10.2 Source continuation

It is possible to use preexisting source particle information for a simulation. The state of the particles within a source at the problem start time can be read from a LODI-compatible netCDF master particle file. This file may be a particle file from a previous simulation or an independently generated file.

10.3 Source emissions

In addition to the source geometry (spatial distribution of mass or activity), the user must specify the time-varying total mass or activity emission rates. This is done by specifying a number of emission times and an emission rate for each of these times. The user must also specify a start time and a stop time that determines the time interval over which a source is active. The input emission rates are assumed to be the average emission rate over the interval and the emission times are the times the corresponding emission rate begins, i.e. for $t_1 \leq t < t_2$ emission rate e_1 will be used while for $t_2 \leq t < t_3$ emission rate e_2 will be used. Note that the first emission rate time must be at the source start time. If emission times are given that are greater than the source stop time they will be ignored. (If emission times greater than the stop time is given, then this can lead to release of fewer computational particles than requested. In this case, the total mass/activity released will be correct. However, fewer computational particles will result in more statistical error.)

11. Aerosol Mass-Size Distributions

The aerosol mass size distribution is the mass (or activity) distribution as a function of aerosol size. It is important to note that this mass size distribution is for the species mass, not necessarily the total mass of the aerosol, which may be a mixture of the species of interest and other materials. The overall particle density (used in the settling velocity calculation) is specified separately from the mass distribution, and is for the total mass of the aerosol. Aerosol size distributions are often reported in terms of *aerodynamic diameter*, defined as the diameter of a unit density (ρ_p = 1 g/cc = 1000 kg/m^3) sphere that has the same settling velocity as the particle. If this is the case, a unit density should be used, which is the code default.

Each source in a simulation may have a different mass size distribution. We allow mass distributions to be specified using either tabular input or via the parameters of a lognormal distribution. An equal number of computational, marker particles are used for each mass distribution bin for both table and lognormal distributions.

Tabular input is useful for representing a variety of mass distributions, particularly, when data on mass fractions in various size intervals are available. When using table input, the user must input (F_n, $d_{n,min}$, $d_{n,max}$) for $n = 1...N$ "mass bins", where F_n is the fraction of the total source mass, $d_{n,min}$ is the minimum diameter, and $d_{n,max}$ is the maximum diameter for bin n. The mass associated with each bin is assumed to be uniformly distributed as a function of diameter in that bin.

Lognormal distributions have been found to describe many single-source aerosol size distributions (Hinds, 1982). The lognormal mass distribution is given by

$$f_{LN}(d_p) = \frac{1}{\sqrt{2\pi}\ln(\sigma_g)} e^{-a} \quad \text{and} \quad a = \left[\frac{\left(\ln(d_p) - \ln(d_m)\right)^2}{2\left(\ln(\sigma_g)\right)^2} \right], \qquad \textbf{(45)}$$

where $f_{LN}(d_p)$ is the fraction of the species mass per unit increment of the logarithm of diameter (i.e., $f_{LN}(d_p)d\ln d_p$ is the fraction of mass on particles with diameter with natural logarithms between $\ln d_p$ and $\ln d_p + d\ln d_p$), d_m is the mass median diameter or MMD, and σ_g is the geometric standard deviation or GSD. (The activity median diameter or AMD is used instead of the MMD for radioactivity or toxicological or biological activity). The user must input MMD (AMD) and GSD for this mass distribution. The lognormal distribution is clipped at the minimum diameter, d_{min}, and maximum diameter, d_{max}, which may be optionally input by the user. The default limits are $d_{min} = \exp(\ln d_m - 4\ln\sigma_g)$ and $d_{max} = \exp(\ln d_m + 4\ln\sigma_g)$. Using the clipped lognormal input parameters, mass distribution bins are generated internally in the code with the width (in units of natural logarithm of diameter) of each bin being equal to $(\ln\sigma_g)/4$.

12. Buoyant Sources

LODI includes parameterizations for the vertical rise of plumes due to initial vertical momentum and/or buoyancy. These parameterizations are based on an integral model that specifies equations for the total fluxes of mass, momentum and thermodynamic energy through a plume cross-section (e.g., Weil, 1988). This model uses several simplifying assumptions that allow analytic expressions for the mean height and radius of the plume as a function of time to be obtained. It is assumed that (1) the difference between the densities of the plume and ambient air is small enough that the Boussinesq approximation is valid $\left((\Delta\rho/\rho << 1\right)$, (2) no internal heat is generated in the plume (e.g., there is no condensation), (3) the pressure in the plume is the hydrostatic value in the ambient, undisturbed atmosphere, (4) the flow is steady-state and incompressible, (5) the plume and ambient air behave as an ideal gas, (6) the plume and ambient air are dry, and (7) the plume properties (e.g., density, velocity) are uniformly distributed across the plume cross section. A key assumption is that the rate of entrainment of ambient air into the plume is proportional to the mean vertical velocity of the plume

(Morton et al., 1956). This implies that the entrainment is due primarily to self-generated turbulence caused by the relative motion of the plume and ambient air. These assumptions are justified by the successful prediction of the observed average stabilized height of plumes in stable atmospheres, and of the near-source rise and spread of plumes (e.g., Briggs, 1975 and 1984).

Assuming that variations in the wind speed and in the vertical temperature gradient can be neglected during plume rise, semi-empirical analytic expressions have been determined for the time-dependent mean vertical rise, $\Delta z_r(t) = z(t) - z_s$ where $z(t)$ is the mean height of the plume and z_s is the initial source height $t = 0$ (e.g., Briggs, 1975; Weil, 1988).

In most cases, either the initial vertical momentum or the initial buoyancy dominates, and expressions for the final rise, Δz_{rf}, have been determined for these cases. In our model, for sources with both initial momentum and initial buoyancy, the final rise due to each effect is calculated separately and the effect yielding the largest final rise is used. However, the final rise of a plume may be limited by several factors, including the intensity of the ambient turbulence and the presence and strength of a stable layers at or above the source. The model calculates limits to the final rise due to these effects independently and imposes the minimum allowed final rise. The expression for the particle trajectory, $\Delta z_r(t)$, corresponding to the dominant process, momentum or buoyancy, is used in order to be consistent with the expression for the final rise. A virtual origin correction accounts for the initial size of the source (Overcamp and Ku, 1986).

The equation $\Delta z_r(t) = \Delta z_{rf}$ is solved analytically to determine the time interval, t_f, to reach the final rise height. For $t \le t_f$ (t here is the "age" of the particle, the time since it was released at the source), an additional term, $w_r = d(\Delta z_r(t))/dt$, is added to mean vertical velocity of the particle due to other processes (mean wind, gravitational settling).

The radius of a plume is assumed to be linearly proportional to the vertical rise, $r(t) = r_0 + \beta' \Delta z_r(t)$. An effective contaminant diffusivity

$$K_r = \left(\sigma_{r_f}^2 - \sigma_{r_0}^2\right) \Big/ 2t_f = \left(\alpha^2 r_f^2 - \alpha^2 r_0^2\right) \Big/ 2t_f$$

where $\alpha = \sigma_r / r$ (the ratio of the standard deviation of the spatial distribution of material in the plume to its radius; the default value is 1/2), is applied to calculate the diffusion of the plume ($K_x = K_y = K_z = K_r$) for $t \le t_f$. Diffusivities due to ambient turbulence are not used during the plume rise phase. (This is a simplification of the actual processes. However, in the derivation of the analytic plume rise equations, plume-generated turbulence is assumed to dominate during the rise, as discussed above).

In the LODI plume rise capability, we use "bent-over" plume equations, which have been studied extensively and are much more developed than vertical plume equations. When plumes have an initial vertical velocity that is small relative to the horizontal ambient wind velocity, they quickly become horizontal (bent over). A different set of equations is used for (a) neutral/unstable and (b) stable static stability conditions in the ambient atmosphere, as discussed below.

12.1 Neutral and unstable conditions

The mean rise, $\Delta z_r(t)$, of a bent-over plume in a uniform horizontal wind and in *neutral* ambient static stability (i.e., $\partial\theta_a/\partial z = 0$, where θ_a is the ambient potential temperature) is calculated using the expression given by Weil (1988). In the unstable boundary layer ($L^{-1} < 0$, $z < h$), the neutral-stability, plume-rise equations are also used, since the mean potential temperature over the bulk of the boundary layer depth is approximately constant (e.g., Wyngaard, 1988).

The final rise, Δz_{rf}, in neutral stability conditions may depend on several factors, including the intensity of the ambient turbulence and the existence of a stable layer above the source height. In neutral and unstable conditions we calculate Δz_{rf} due to both ambient turbulence and the elevated stable layer at the top of the boundary layer, and use the minimum of these values.

Using an expression developed by Berkowicz et al. (1986), the final rise height of a buoyancy-dominated plume is limited by an overlying stable layer at $(z - z_g) \geq h$ when the initial source height, z_s, is below the top of the boundary layer height (i.e., $(z_s - z_g) < h$). In the neutral or unstable boundary layer ($z - z_g < h$, $L^{-1} \leq 0$), the maximum rise of a buoyancy-dominated plume due to ambient mechanically-generated turbulence is calculated using the expression given by Weil (1988; from a Briggs private communication). In the unstable ABL ($z - z_g < h$, $L^{-1} < 0$), the maximum rise of a buoyancy-dominated plume due to small-scale ambient buoyancy-generated turbulence is calculated using the expression given by Briggs (1984), and for large-scale ambient buoyancy-generated turbulence is calculated using the expression given by Weil and Hoult (1973). The Weil and Hoult expression was determined by assuming that plume rise is effectively ended when the plume vertical velocity is equal to the standard deviation of the ambient vertical velocity.

We use an equivalent expression for momentum-dominated plume rise limited by large-scale buoyancy-generated turbulence in the unstable ABL. For a momentum-dominated plume in the unstable ABL ($z < h$, $L^{-1} < 0$), the final rise limited by small-scale ambient buoyancy-generated turbulence is calculated using the expression given by Briggs (1984). For a non-buoyant plume (momentum rise only) with $z_s < h$ the maximum rise in neutral or unstable conditions is assumed to also be limited by a capping inversion at the boundary layer height, i.e., $\Delta z_{rf} = h - z_s$.

12.2 Stable conditions

The mean rise, $\Delta z_r(t)$, of a bent-over plume in a uniform horizontal wind and in *stable* ambient static stability ($\partial\theta_a/\partial z > 0$ and assumed constant) is calculated using the expression given by Weil (1988). The final rise, Δz_{rf}, of bent-over plumes in stable conditions is the maximum of the buoyancy-dominated final rise and the momentum-dominated final rise expression given by Briggs (1975).

Plume rise in stable conditions depends on the ambient potential temperature gradient, $\partial\theta_a/\partial z$, which is determined ($z < h, L^{-1} > 0$) using the following surface layer similarity theory relationship:

$$\frac{\partial\theta_a}{\partial z} = \frac{\theta_*}{kz}\phi_h\left(z/L\right)$$

where

$$\theta_* = \frac{u_*^2 T_a}{kgL}$$

and

$$\phi_h(z/L) = 1 + 5\frac{z}{L}$$

As discussed by Venkatram (1988), this can be a reasonable approximation for the entire depth of the stable boundary layer. For $z > h$, the standard atmosphere temperature gradient, $\partial T_a / \partial z = -0.0065$ Km^{-1}, is used to calculate a value for $\partial \theta_a / \partial z$.

13. Concentrations

13.1 Air concentration types

LODI provides four different mean air concentration types: instantaneous, time-averaged, peak averaged, and integrated. The instantaneous air concentration is the mean concentration at a location at time *t*. The time-averaged air concentrations are defined by:

$$\overline{AC}(x,y,z,t) = \frac{\int_{t-\Delta t}^{t} \overline{C}(x,y,z,t')dt'}{\Delta t} \quad . \qquad \textbf{(46)}$$

The peak averaged air concentrations are defined by:

$$\overline{PC}(x,y,z,t) = \max_{i=l,n}\left[\frac{\int_{t-(n-i+1)\Delta t}^{t-(n-i)\Delta t} \overline{C}(x,y,z,t')dt'}{\Delta t}\right]. \qquad \textbf{(47)}$$

The integrated air concentrations are defined by:

$$\overline{IC}(x,y,z,t) = \int_{t-\Delta t}^{t} \overline{C}(x,y,z,t')dt' \quad . \qquad \textbf{(48)}$$

For averaged and integrated air concentrations, the user specifies both the interval between output times, *t*, and the sampling period, Δt. Thus it is possible to obtain a one hour integrated concentration at every hour or a one hour integrated concentration every three hours. The only restriction is that the integration period must be less than the interval between outputs, i.e. hour integrated concentrations every fifteen minutes cannot be produced. For peak averaged air concentration, the user again specifies the sampling time, Δt, and the interval between output times. However, the interval between output times must be an integer multiple of Δt. Thus the user can request the peak 5 minute average concentration for every hour, but not the peak 10 minute average every 25 minutes.

13.2 Air concentration sampling

There are three distinct sampling geometries available within LODI for the calculation of air concentrations: three-dimensional, quasi-two-dimensional "horizontal", and quasi-two-dimensional vertical. A three-dimensional sampling bin contains a three-dimensional array (x, y, σ_z) of mean concentration values at the centroid of each grid box within the concentration grid (the sampling volumes are the cells of the concentration grid).

To minimize storage or to yield a mean concentration at a specific position, it is usually convenient to request a quasi-two-dimensional "horizontal" sampling geometry. In this case, the sampling area in the (x, y) plane is determined by the (x, y) projection of the concentration grid. The sampling depth in the z direction and the height of the sampling plane is specified by the user. For example, the user may request a "horizontal" sampling volume at a height of 1500 meters with a sampling depth of 40 meters. The sampling volumes will have the horizontal cell structure of the concentration grid and extend from 1480 to 1520 meters in the vertical. The result is a two-dimensional array (x, y) of concentration values at the cell centers of the (x, y) concentration grid. It is possible to request that the sampling height be interpreted as either height above mean sea level or as height above ground.

There are three caveats that the user must be aware of when specifying this geometry. The first is that if the user specifies a very small sampling depth compared to the number of particles released the sampling statistics will be unreliable because the probability of any particle being in such a small volume will be small. The second is that if the user requests a sampling height of 10 meters AGL (Above Ground Level) and a sampling depth of 40 meters, LODI will override the 10 meter height and move it to, in this case, 20 meters to avoid trying to sample below ground. When a bin position is modified a warning message is written to "standard out" to alert the user. In contrast, if a sampling height is specified as height MSL (above Mean Sea Level), no allowance for terrain is made and parts of the sampling volumes may be under ground if a user requests a height below the maximum terrain elevation in the grid.

In addition to the quasi-two-dimensional "horizontal" sampling geometry there is a corresponding quasi-two-dimensional vertical sampling geometry. In this case, the user specifies a location either in x or y and a sampling width. The sampling volumes will be determined by the concentration grid projection in the (y, σ_z) plane if a constant x is specified or in the (x, σ_z) plane if a constant y is specified; with a width in the perpendicular direction centered on the location. If the user requests a sampling location and a sampling width such that the sampling location ±½ the sampling width is outside of the sampling grid domain, the sampling location will be moved to the grid limit ±½ the sampling width, and a warning message is written to "standard out". As before, the user must be aware of the relationship between sampling width and number of particles used in a simulation. It is not currently possible to request a vertical sampling volume that crosses the coordinate lines at an angle.

13.3 Moving receptor capability

In addition to static sampling bins, LODI has a moving receptor capability. This capability allows users to specify one or more receptors that move through the problem domain and accumulate concentrations. The moving receptor is a quadrilateral volume that is treated either as a single sampling volume or divided into equal sized smaller sampling volumes that move together (Figure 5). The movement of the receptors can be specified as in either MSL or AGL coordinates. As with static sampling bins, if the specified receptor width and initial center location cause some of the receptor to be below ground the center is moved up until the receptor is above ground. These receptors can be used to simulate a single vehicle or a group of vehicles moving together. As with moving sources, the receptor motion is specified by the user via a list of times and positions of the volume center. The receptors are then moved by using linear interpolation in time to calculate a new center location. Currently, integrated, interval average, peak average or instantaneous air exposure can be calculated.

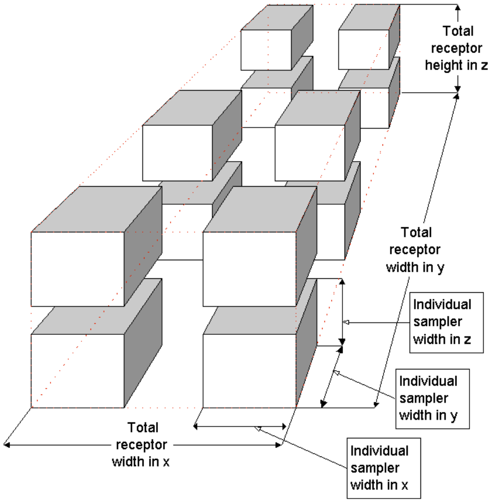

Figure 5. Receptor example with a 2 x 3 x 2 set of sampling volumes.

There are four cautions the user should be aware of when using this option. First, it can be computationally expensive because the particle time steps are restricted by the closing speed between the particles and the receptors which can be significantly larger than the particle speed. Second, only the region at the receptor center is checked to assure it is above ground. Therefore a horizontally large receptor may be partially below ground near a steep rise in terrain. Third, there is no check that the receptor moving in MSL coordinates does not run into or though the surface. Fourth, the user must assure that the receptor volume and number of particles in the sampling region are sufficient to give statistically correct values.

13.4 Deposition

All deposition calculations are done on the ground surface. Thus all deposition bins are two-dimensional "horizontal" bins and the sampling areas are determined by the (x,y) projection of the concentration grid at $\sigma_z = 0$.

There are a number of different deposition concentration fields which are categorized by process (dry or wet deposition) and by type (accumulated deposition or time integrated exposure). Accumulated deposition at time *t* is calculated by summing the contributions of all particles to the deposition in each surface grid cell from time *tstart* to time *t*.

$$D(x,y,z,t) = \int_{tstart}^{t} j_d(x,y,z,t')dt' \qquad \textbf{(49)}$$

where j_d is the deposition flux as a function of time and position. Integrated deposition exposure, ID, over a time period Δt (Δt must be the interval between output times) is needed for external, ground-exposure radioactive dose calculations and is defined as follows:

$$ID(x,y,z,t) = \int_{t-\Delta t}^{t} D(x,y,z,t')dt' \ . \qquad \textbf{(50)}$$

The decay of previously deposited material is accounted for in both the accumulated deposition and integrated deposition exposure calculations, but is not shown in the previous two equations.

Output of accumulated deposition, *D*, and integrated deposition exposure, *ID*, are requested for wet deposition and dry deposition separately.

14. Files

14.1 Input

To execute LODI, several input files must exist (see Figure 6). At the start of execution, LODI reads two ASCII files containing FORTRAN90 name lists: "lodi.nml" and "lodi_files.nml". These files contain the various options and parameters needed to complete a simulation. The contents of these files are described in more detail in Section 15.

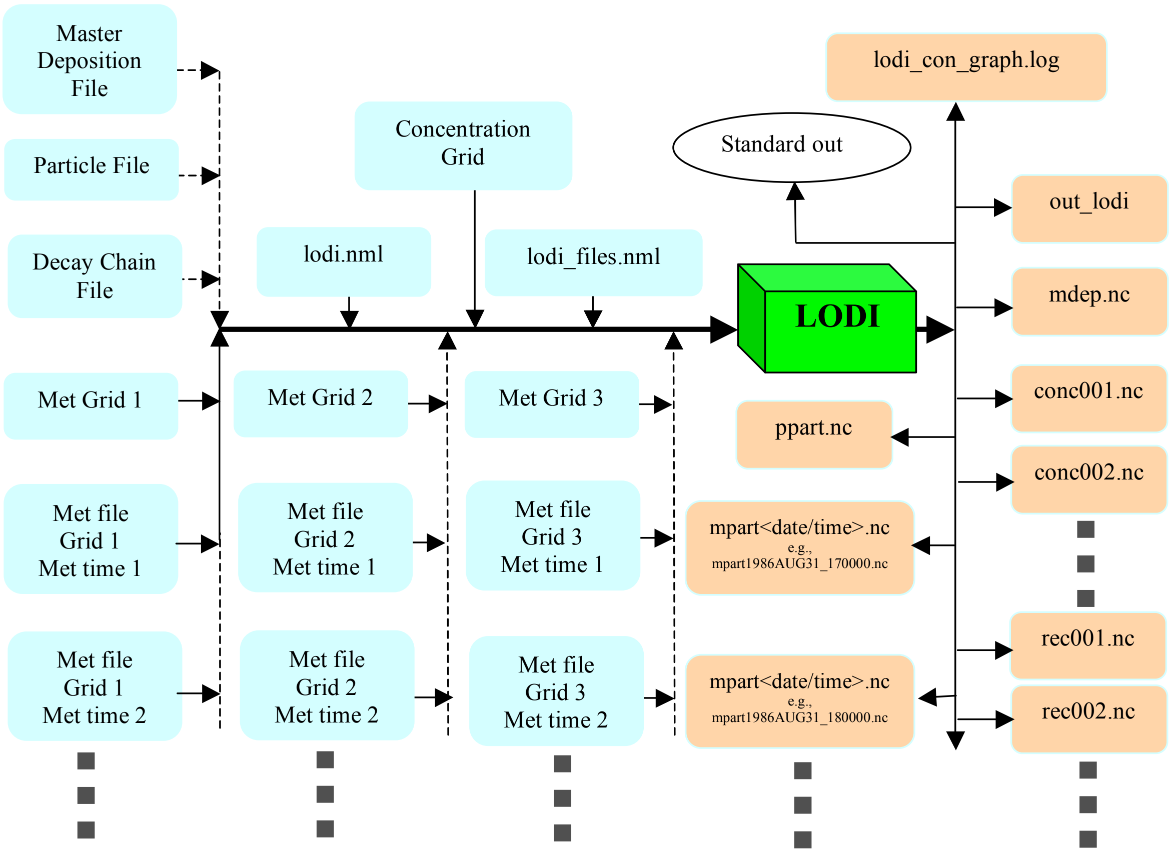
Master Deposition File
Particle File
Decay Chain File
Concentration Grid
lodi.nml
lodi_files.nml
LODI
Standard out
lodi_con_graph.log
out_lodi
mdep.nc
conc001.nc
conc002.nc
ppart.nc
rec001.nc
rec002.nc
Met Grid 1
Met Grid 2
Met Grid 3
Met file Grid 1 Met time 1
Met file Grid 2 Met time 1
Met file Grid 3 Met time 1
Met file Grid 1 Met time 2
Met file Grid 2 Met time 2
Met file Grid 3 Met time 2
mpart<date/time>.nc e.g., mpart1986AUG31_170000.nc
mpart<date/time>.nc e.g., mpart1986AUG31_180000.nc

Figure 6. LODI file I/O. (Note that input files connected with solid line represent the minimum set necessary to execute a simulation.)

Besides the namelist files, netCDF grid files are required which describe each of the meteorological data grids. Also required is a netCDF grid file describing the concentration grid to be used in the simulation. These files must conform to the NARAC standard grid file format.

The model requires a meteorological data file for each meteorological data time and each meteorological data grid. These files must be netCDF files that meet the specification for NARAC gridded met data files as described in the ADAPT User's Manual. These files provide the gridded mean wind components $(\overline{u},\overline{v},\overline{w})$, and turbulence parameter fields, K_z, σ_v^2, t_L, u_*, L^{-1}, and boundary layer height.

If the user wishes to specify individual particle locations for a source or continue a previous simulation, a netCDF file containing the necessary particle parameters such as location, mass, age, and diameter is also required. This file must conform to the LODI master particle file format as defined in this manual. For a continuation run, this file should be the appropriate mpart<date/time>.nc file from the run being continued. If a simulation which involves deposition is being continued, the master deposition file must also be available as input. This file must conform to the NARAC master deposition file format and should be the mdep.nc file output during the run being continued.

If the user wishes to simulate radioactive decay chains, a copy of the decay chain database must be available. This file is available from the Radiation Shielding Information Center, Oak Ridge, Tennessee as data set DLC-80/DRALIST (ORNL, 1980).

14.2 Output

LODI produces a number of different output files. The most important of these files are the netCDF concentration files, "concxxx.nc" where xxx are sequential numbers. A concentration file contains the requested concentrations for a single concentration bin at all of the requested bin output times. If the moving receptor option is activated there will be one netCDF receptor file, "recxxx.nc" where xxx are sequential numbers for each active receptor. These files contain the accumulated air concentrations and center locations for each of the receptor sampling volumes, for all requested receptor output times.

For graphics purposes the netCDF particle file, "ppart.nc" is output containing the particle positions as a function of time for a user specified set of particles.

For run continuation purposes, the netCDF master particle files mpart<date/time>.nc, where <date/time> is the file valid time in NARAC time string format, are output. These files contain all the information associated with a particle for all the particles in a simulation at each of the requested dump times. There is one master particle file for each requested time. This file can be used as an input file describing a source for a continuation simulation. For simulations which include deposition, the master deposition file, "mdep.nc", is also written. This file contains the deposition data necessary to continue a simulation.

In addition to the netCDF output files, LODI produces an ASCII log file, "out_lodi", that contains an echo of the input namelists. On request, this file can also contain either particle locations at each particle dump time, concentration bin output for each bin output time, or both for debugging and testing. A small ASCII concentration bin vs file name log, "lodi_con_graph.log", is also written. Finally, LODI writes ASCII status messages to "standard out" during execution.

14.3 Output netCDF Sample Headers

14.3.1 Concentration file

The following is a cdl list of the header information in the concentration file for a 2D horizontal bin which output hour averaged concentrations at each hour interval.

```
netcdf conc001 {
dimensions:
        elapsed_time = UNLIMITED ; // (3 currently)
        nspec = 1 ;
        gr1 = 50 ;
        gr2 = 50 ;
        zt_dim = 1 ;
        dim40 = 40 ;
        num_srcdim = 2 ;
        cgridx = 51 ;
        cgridy = 51 ;
variables:
        char start_time_str(elapsed_time, dim40) ;
        char stop_time_str(elapsed_time, dim40) ;
        char source_list(num_srcdim, dim40) ;
        char species_name(nspec, dim40) ;
        double elapsed_time(elapsed_time) ;
                elapsed_time:long_name = "Sampling_Time" ;
                elapsed_time:units = "Seconds" ;
                elapsed_time:selection_category = "NULL" ;
        double concen(elapsed_time, gr1, gr2) ;
                concen:long_name = "Average Concentration" ;
                concen:units = "units/m3" ;
                concen:plane_type = 1 ;
        double gr1(gr1) ;
                gr1:long_name = "x       " ;
                gr1:units = "meters" ;
                gr1:selection_category = "NULL" ;
        double gr2(gr2) ;
                gr2:long_name = "y       " ;
                gr2:units = "meters" ;
                gr2:selection_category = "NULL" ;
        double zt(zt_dim) ;
        double area_cell(gr1, gr2) ;
        double cgridx(cgridx) ;
                cgridx:long_name = "xgr" ;
                cgridx:units = "meters" ;
        double cgridy(cgridy) ;
                cgridy:long_name = "ygr" ;
                cgridy:units = "meters" ;
        double zgij(gr1, gr2) ;

// global attributes:
                :title = "LODI Test                                                                       " ;
                :bin_id = "Bin 1-Avg. xy 0-20m AGL                 " ;
                :sampling_type = "average                 " ;
                :sampling_interval = 3600. ;
                :create_file = "conc001.nc                                                                      " ;
                :create_code = "LODI" ;
                :create_version = "version 0.91 2001Apr10  " ;
                :create_type = "concentration data" ;
                :grid_id = "GridGen_conc_sigmaZ_plane_UTM_vertgridpt_-99999_-
99999_51_51_31_40000_40000_1_711000_3895100_1999JUL21_092223                                                   " ;
                :type = "air                     " ;
                :orientation = "xy      " ;
                :create_date_time = "2001APR10_184205                        " ;
                :problem_start_time = "1986AUG31_150000                        " ;
                :position = 10. ;
                :width = 20. ;
                :bin_agl_flg = "AGL     " ;
}
```

14.3.2 Particle position file

The following is a cdl list of the header information in the particle position file.

```
netcdf ppart {
dimensions:
        elapsed_time = UNLIMITED ; // (6 currently)
        pnum = 10000 ;
        dimnum = 3 ;
        dim12 = 12 ;
        nsrc = 3 ;
        dim40 = 40 ;
variables:
        char time_str(elapsed_time, dim40) ;
        double elapsed_time(elapsed_time) ;
                elapsed_time:long_name = "Time" ;
                elapsed_time:units = "sec" ;
                elapsed_time:selection_category = "NULL" ;
        long dimnum(dimnum) ;
                dimnum:long_name = "Cartesian Coordinate" ;
                dimnum:coord_labels = "dimnum_labels" ;
                dimnum:selection_category = "NULL" ;
        char dimnum_labels(dimnum, dim12) ;
                dimnum_labels:selection_category = "NULL" ;
        long nsrc(nsrc) ;
                nsrc:long_name = "Number of Sources" ;
        char sourceid(nsrc, dim40) ;
                sourceid:long_name = "List of Sources" ;
        double part_posn(elapsed_time, nsrc, pnum, dimnum) ;
                part_posn:long_name = "Particle Positions" ;
                part_posn:units = "Meters" ;
                part_posn:fill_value = -99999. ;
        long in_grid(elapsed_time, nsrc, pnum) ;
                in_grid:long_name = "Particle Flag to Determine if in Grid" ;
                in_grid:fill_value = 0 ;

// global attributes:
                :title = "LODI Test                                                                       " ;
                :create_file = "part.nc" ;
                :create_code = "LODI" ;
                :create_version = "version 0.91 2001Apr10  " ;
                :create_type = "particle data" ;
                :create_date_time = "2001APR10_184205                        " ;
}
```

14.3.3 Master particle file

The following is a cdl list of the header information in the master particle file.

```
netcdf mpart1986AUG31_160000 {
dimensions:
        elapsed_time = 1 ;
        pnum = 20000 ;
        dimnum = 3 ;
        dim12 = 12 ;
        nsrc = 3 ;
        dim24 = 24 ;
        dim40 = 40 ;
        nspec = 1 ;
variables:
        char time_str(dim40) ;
                time_str:long_name = "Time string" ;
        double elapsed_time(elapsed_time) ;
                elapsed_time:long_name = "Time" ;
                elapsed_time:units = "sec" ;
                elapsed_time:selection_category = "NULL" ;
        long dimnum(dimnum) ;
                dimnum:long_name = "Cartesian Coordinate" ;
                dimnum:coord_labels = "dimnum_labels" ;
                dimnum:selection_category = "NULL" ;
        char dimnum_labels(dimnum, dim12) ;
        long nsrc(nsrc) ;
                nsrc:long_name = "Number of Sources" ;
        char sourceid(nsrc, dim40) ;
                sourceid:long_name = "List of Sources" ;
        char species_name(nsrc, nspec, dim40) ;
                species_name:long_name = "Species Names" ;
        long num_spec(nsrc) ;
                num_spec:long_name = "Number of Species per Source" ;
        long mx_npart(nsrc) ;
                mx_npart:long_name = "Maximum Number of Particles per Source" ;
        long num_part(nsrc) ;
                num_part:long_name = "Number of Particles Generated per Source" ;
        long in_grid(nsrc, pnum) ;
                in_grid:long_name = "Particle Flag to Determine if in Grid" ;
                in_grid:fill_value = 0 ;
        double age_part(nsrc, pnum) ;
                age_part:long_name = "Particle Age" ;
                age_part:units = "sec" ;
                age_part:fill_value = -99999. ;
        double part_posn(nsrc, pnum, dimnum) ;
                part_posn:long_name = "Particle Positions" ;
                part_posn:units = "Meters" ;
                part_posn:fill_value = -99999. ;
        double mass_part(nsrc, pnum, nspec) ;
                mass_part:long_name = "Particle Mass" ;
                mass_part:fill_value = -99999. ;
        double inimass_part(nsrc, pnum, nspec) ;
                inimass_part:long_name = "Particle Initial Mass" ;
                inimass_part:fill_value = -99999. ;
        double diam_part(nsrc, pnum) ;
                diam_part:long_name = "Particle Diameter" ;
                diam_part:units = "Meters" ;
                diam_part:fill_value = -99999. ;
        double density_part(nsrc, pnum) ;
                density_part:long_name = "Particle Density" ;
                density_part:units = "kg/m**3" ;
                density_part:fill_value = -99999. ;
        char incloud_part(nsrc, pnum, dim24) ;
                incloud_part:long_name = "Particle Buoyancy Type" ;

// global attributes:
                :title = "LODI Test                                                                       " ;
                :create_file = "part.nc" ;
                :create_code = "LODI" ;
                :create_version = "version 0.91 2001Apr10  " ;
                :create_type = "particle data" ;
                :create_date_time = "2001APR10_184500                        " ;
}
```

15. LODI Input NameLists Descriptions

Table 1. Namelists in file lodi.nml in the order they are read.

Namelist name	Use
prob_setup	To input global problem variables.
thist_param	*to be implemented (tbi).*
src_param	To define individual sources. *There must be a src_param namelist for each source.*
bin_param	To define individual sampling bins. *There must be a bin_param namelist for each sampling bin.*
turb_param	To define the various K models to be used and the parameters necessary for the K models.
met_param	To define various meteorological parameters necessary to run the model.
receptor_param	To define the individual moving receptors. *There must be a receptor_param namelist for each moving receptor.*

Table 2. Namelists in file lodi_files.nml in the order they are read.

Namelist name	Use
grid_name	To link problem grid files to code.
metfiles	To list problem meteorological data file names input to code. *There must be a metfiles namelist for each grid used in a simulation*.
decay_chains_file	To allow decay chain constants to be read.
particle_file	To allow particles generated previously to be read as part of a source
dep_files	To allow continuation of deposition calculations from a previous simulation.

15.1 Namelists contained in the file 'lodi.nml'

For notational simplicity, the following convention is followed in the namelist descriptions. If a namelist variable is a character value that refers to a numerical value, e.g. tstart_str which is a character variable which refers to a time, the numeric value of that variable will be referred to as the namelist variable name without the "_str". Thus tstart > tstop refers to the numeric values not the character values of tstart_str and tstop_str.

Table 3. Namelist prob_setup contents (lodi.nml)

prob_setup		
Variable Name	Descriptions and Possible Values	Default
title	Character (80) string used as title of simulation	
tstart_str	The simulation starting time *NARAC date/time string format "1997JAN01_hhmmss"*	
tstop_str	The simulation stop time *NARAC date/time string format "1997JAN01_hhmmss"*	
rd_grid	Character (8) string indicating type of meteorological data grid file input "ascii" => read ASCII format file "gridgen" => read GRIDGEN grid file *Note: ascii format should only be used by developers or specialized research conditions*	"gridgen"
met_format	Character (8) string indicator of the format of the meteorological data file. "arac" => use Arac-3 netCDF gridded data standard "gtx" => use older GTX data format *Note: gtx format should only be used by developers on data generated before 28 April 1997.*	"arac"
num_met_times	Integer number of meteorological data sets to be used. (Valid choices 1-200)	
met_time_strs	1D array of length "num_met_times" of valid times for the meteorological data sets *NARAC date/time string format "1997JAN01_hhmmss"*	
dt_limit	Largest time step allowed during the simulation in seconds	3600.0

prob_setup		
Variable Name	Descriptions and Possible Values	Default
dt_min	Minimum particle time step to use during the simulation in seconds	0
dt_fact_adv	Factor multiplying the calculated advection time step *Note, should be used by developers only.*	1.0
dt_fact_dif	Factor multiplying the calculated diffusion time step *Note, should be used by developers only.*	1.0
dt_part_str	Character (40) string indicating the time interval between particle information output dumps to the particle position file ppart.nc. String format is "days::hours:minutes:seconds", where days is the integer number of days, hours is the integer number of hour, minutes is an integer number of minutes, and seconds is the floating point number of seconds. Since the string is interpreted from the right leading units may be omitted, i.e. "200.5" is interpreted as 200.5 seconds, "10:5" is interpreted as 10 minutes and 5 seconds. All separators to the right must be entered, i.e. "2:0" or "2:" is interpreted as 2 minutes, "2::0:0:0" or "2::::" is interpreted as 2 days. To prevent any output to this particle position file, enter a values of "0::00:00:00"	
dt_dump_str	Character (40) string indicating the time interval between master particle information output to the files, 'mpart<date/time/string>.nc' and to the master deposition file, 'mdep.nc,' These files are necessary for restarting a simulation with data from this simulation. *Note: dt_dump_str must be an integer multiple of dt_part_str.* String format is "days::hours:minutes:seconds", where days is the integer number of days, hours is the integer number of hour, minutes is an integer number of minutes, and seconds is the floating point number of seconds. To prevent any output to these file, enter a values of "0::00:00:00"	
npart_pos	Integer number of particles to output to the particle position file ppart.nc	
out_bin_ascii	Logical indicator for ascii data dumps of concentration bin in file out_lodi. .true. => write ascii dumps .false. => do not write ascii dumps	.false.
out_part_ascii	Logical indicator for ascii data dumps of particle positions in file out_lodi. .true. => write ascii dumps .false. => do not write ascii dumps	.false.

prob_setup		
Variable Name	Descriptions and Possible Values	Default
solver_id	Character (8) indicator of which advection scheme to use "rk2" => use second order Runge-Kutta scheme	"rk2"
rdm_dist	Character (8) indicator of the type of distribution to be used for the diffusive displacements "gauss" => Gaussian distribution "nongauss" => Non Gaussian distribution	"nongauss"
minmass_frac	Minimum mass fraction (current mass divided by initial mass) used as criteria to eliminate a particle from the simulation	1.0e-06
reflect	Character (8) indicator of the reflection method used for particles that go below ground "none" => do not reflect "vertical" => reflect particles below ground level by setting σ_z to $\left|\sigma_z\right|$ while leaving x and y the same "vertztop" => reflect particles below ground in same manner as if reflect = "vertical", AND, if σ_z coordinate is above grid top, then reflect particle to new position σ_z = 2*sigmaz_top - σ_z.	"vertical"
dz_dep	Height in meters of the absorbing layer used to calculate dry deposition	20
nsrc	Integer number of sources to be defined. *There must be nsrc src_param namelists contained in the input file.*	1
nbins	Integer number of output bins to be defined. *There must be nbins bin_param namelists contained in the input file.*	
nreceptors	Integer number of moving receptors to be defined	0
slip_factor	Calculate the surface slip velocity as a factor times the velocity at the first point above the surface, i.e. u(i, j, 1) = slip_factor * u(i, j, 2) Note: *This is for use when wind data is passed directly from COAMPS (and not through ADAPT).*	1.0
dt_constant	Constant time step (overrides all other values.) *Note, should be used by developers only.* 0 => use code calculated variable time step non-zero implies use this value as constant time step	0
out_debug_param	Logical flag to specify if turbulence and plume rise debug arrays are to be written to files.	.false.

Table 4. Namelist thist_param contents (lodi.nml) *(Note: This namelist is currently unused. However, a blank namelist with this name must be present for LODI to run)*

Variable Name	Descriptions and Possible Values	Default

Table 5. Namelist src_param contents (lodi.nml)

<table>
<tr><th colspan="3">src_param</th></tr>
<tr><th>Variable Name</th><th>Description and possible values</th><th>Defaults</th></tr>
<tr><td>source_id</td><td>Character (40) string to identify this source.</td><td></td></tr>
<tr><td>start_time_str</td><td>The time that emissions from this source begin.
NARAC date/time string format “1997JAN01_hhmmss”
(start_time must be ≥ tstart)</td><td></td></tr>
<tr><td>stop_time_str</td><td>The time that emissions from this source stop.
NARAC date/time string format “1997JAN01_hhmmss”</td><td></td></tr>
<tr><td>source_model</td><td>Character (24) string indicating buoyancy model to be used for this source.
“neutral” => source is neutrally buoyant with no initial momentum
“plume rise” => analytic momentum and/or buoyant plume rise for a continuous sources is calculated
Note: source_model = “plume rise” assumes a horizontal circular area source (geom_type = 5) and therefore, the following parameters are necessary: x_center, y_center, z_center, radius</td><td>“neutral”</td></tr>
<tr><td colspan="3">Parameters for source_model = “plume rise”
The following input parameter combinations are valid for plume rise:
1) heat_emiss_rates *alone (no momentum contribution to plume rise)*
2) vert_vel *alone (no buoyant contribution to plume rise)*
3) vert_vel, temp *and (optionally)* temp_ambient
*(*heat_emiss_rates ignored if temp input)
4) vert_vel *and* heat_emiss_rates</td></tr>
<tr><td>vert_vel</td><td>1D array of initial vertical velocities of the admixture of source material and air in m/s at each time given in geom_time_str. Used to calculate the initial momentum flux and (with temp) the initial buoyancy flux. Required input for sources with initial vertical momentum.</td><td></td></tr>
</table>

src_param

Variable Name	Description and possible values	Defaults
temp	1D array of initial temperatures (Kelvin) of the admixture of source material and air at each time given in geom_time_str. Used (along with vert_vel and temp_ambient) to calculate the initial buoyancy flux.	
temp_ambient	1D array of ambient air temperatures (Kelvin) at the source location and height at each time given in geom_time_str. Used with vert_vel and temp to calculate the initial buoyancy flux.	288.15
heat_emiss_rates	1D array of sensible heat emission rates for source in Watts (W) at each time given in geom_time_str. Optional parameter used instead of temp to calculate the initial buoyancy flux. Only used if temp values are not entered.	
max_plume_rise	1D array of maximum plume rise heights (m AGL) at each time given in geom_time_str. It is measured from the ground to the maximum height of the top of the plume. *Note: if max_plume_rise is not set the calculated plume rise will be used without an upper limit.*	
End parameters for source_model = “plume rise”		
src_generation_method	Generation method for this source ‘new’ => a new source ‘continuation’ =>a continuation of a source previously started via either an external model or previous simulation. *Note: The continuation option requires a file containing the source particle information, and is indicated via an entry in the particle_file namelist. If deposition has been calculated, a file containing the deposition information is required, and is indicated via an entry in the dep_file namelist.*	‘new’

src_param		
Variable Name	Description and possible values	Defaults
geom_type	Integer indicator of source geometry. 1 => line source 2 => Gaussian source 3 => point source 4 => spherical source 5 => horizontal circular area source (infinitesimally thin in the vertical direction)	2
max_num_part	Integer total number of particles to be released from this source. (For src_generation_method = ‘continuation’ this is the number of new particles to be generated during this simulation.)	
geom_time_strs	1D character (40) array containing the valid times for the source geometry variables. *(Maximum number is 50)* *NARAC date/time string format “1997JAN01_hhmmss”* *(start_time must be ≥ the value of the first geom_time)* *Note: geom_time_strs is reinitialized after each source_param namelist is read.*	
src_agl_flg	Logical flag indicating whether the source geometry z values are to be interpreted as height above mean sea level (MSL) or height above ground level (AGL). .true. => z is AGL .false. => z is MSL	.true.
Geometric parameters for a line source (geom_type = 1)		
x1	1D array containing the x coordinate in meters of the beginning of the line source at each time listed in geom_time_strs.	0
y1	1D array containing the y coordinate in meters of the beginning of the line source at each time listed in geom_time_strs.	0

src_param

Variable Name	Description and possible values	Defaults
z1	1D array containing the z coordinate in meters of the beginning of the line source at each time listed in geom_time_strs.	0
x2	1D array containing the x coordinate in meters of the end of the line source at each time listed in geom_time_strs.	0
y2	1D array containing the y coordinate in meters of the end of the line source at each time listed in geom_time_strs.	0
z2	1D array containing the z coordinate in meters of the end of the line source at each time listed in geom_time_strs.	0
Geometric parameters for a Gaussian Source (geom_type = 2)		
mean_x	1D array containing the x coordinate in meters of the mean of a Gaussian source at each time listed in geom_time_strs.	0
mean_y	1D array containing the y coordinate in meters of the mean of a Gaussian source at each time listed in geom_time_strs.	0
mean_z	1D array containing the z coordinate in meters of the mean of a Gaussian source at each time listed in geom_time_strs.	0
std_x	1D array containing the standard deviation in meters in the x direction for Gaussian sources at each time listed in geom_time_strs.	1
std_y	1D array containing the standard deviation in meters in the y direction for Gaussian sources at each time listed in geom_time_strs.	1
std_z	1D array containing the standard deviation in meters in the z direction for Gaussian sources at each time listed in geom_time_strs.	1
cutoff_dx_min	1D array of positive distance in meters from the x mean position to minimum cutoff value for the Gaussian source at each time listed in geom_time_strs, i.e. for x < (mean_x - cutoff_dx_min) the Gaussian distribution will be cutoff.	

src_param

Variable Name	Description and possible values	Defaults
cutoff_dx_max	1D array of positive distance in meters from the x mean position to maximum cutoff value for the Gaussian source at each time listed in geom_time_strs, i.e. for x > (mean_x + cutoff_dx_max) the Gaussian distribution will be cutoff.	
cutoff_dy_min	1D array of positive distance in meters from the y mean position to minimum cutoff value for the Gaussian source at each time listed in geom_time_strs, i.e. for y < (mean_y - cutoff_dy_min) the Gaussian distribution will be cutoff.	
cutoff_dy_max	1D array of positive distance in meters from the y mean position to maximum cutoff values for the Gaussian source at each time listed in geom_time_strs, i.e. for y > (mean_y + cutoff_dy_max) the Gaussian distribution will be cutoff.	
cutoff_dz_min	1D array of positive distance in meters from the z mean position to minimum cutoff value for the Gaussian source at each time listed in geom_time_strs, i.e. for z < (mean_z - cutoff_dz_min) the Gaussian distribution will be cutoff.	
cutoff_dz_max	1D array of positive distance in meters from the z mean position to maximum cutoff value for the Gaussian source at each time listed in geom_time_strs, i.e. for z > (mean_z + cutoff_dz_max) the Gaussian distribution will be cutoff.	
angle_deg	The angle in degrees counter-clockwise from the x axis to rotate the Gaussian source. (0 ≤ angle_deg ≤ 90)	0
Geometric parameters for a point source (geom_type = 3)		
x_pt	1D array of x coordinates in meters for a point source at each time listed in geom_time_strs.	0

src_param		
Variable Name	Description and possible values	Defaults
y_pt	1D array of y coordinates in meters for a point source at each time listed in geom_time_strs.	0
z_pt	1D array of z coordinates in meters for a point source at each time listed in geom_time_strs.	0
Geometric parameters for a spherical source (geom_type = 4)		
x_center	1D array containing the x coordinate in meters of the source center for spherical sources at each time listed in geom_time_strs.	0
y_center	1D array containing the y coordinate in meters of the source center for spherical sources at each time listed in geom_time_strs.	0
z_center	1D array containing the z coordinate in meters of the source center for spherical sources at each time listed in geom_time_strs.	0
radius	1D array containing the radius in meters of spherical sources at each time listed in geom_time_strs.	1
Geometric parameters for a circular area source (geom_type = 5)		
x_center	1D array containing the x coordinate in meters of the source center for circular area sources at each of the geom_time.	0
y_center	1D array containing the y coordinate in meters of the source center for circular area sources at each of the geom_time.	0
z_center	1D array containing the z coordinate in meters of the source center for circular area sources at each of the geom_time.	0
radius	1D array containing the radius in the horizontal (x,y) plane of circular area sources at each time listed in geom_time_strs.	1

src_param		
Variable Name	Description and possible values	Defaults
End of geometric parameters		
er_time_strs	1D character (40) array of valid start times for source emission rates. *(Maximum number is 50)* *NARAC date/time string format "1997JAN01_hhmmss"* *(start_time must be ≥ the first er_time)* *Note: er_time_strs is reinitialized after each source_param namelist is read.*	
er_units_type	Character (24) string specifying whether the emission rates are in activity or mass units. "mass" => units of mass/time, e.g. kg/s "radioactivity" => units of activity/time, e.g. Ci/s	"radioactivity"
emiss_rates	2D array of emission rates in (mass or activity units)/s starting at each of the er_times (Emission rate held constant until next er_time) for each species Dimension = (no. of er_times, no. of species)	0
species	1D array of character (40) strings identifying the radioactive or chemical species associated with this source. Note: The first 8 characters of the string must match the name in the radioactive decay chain constants database specified in the decay_chains_file namelist. For all radioactive species, the first 3 to 7 characters must be in the format "ee-aaam" where "ee" is the one or two character element identifier, "aaa" is the one to three character atomic weight of the isotope, and "m" is a single character indicating metastable state. Valid examples are H-3, Y-90M, I-133, XE-133, and XE-133M . Maximum number = 100	

src_param		
Variable Name	Description and possible values	Defaults
mass_distrib	Character (24) string identifying how mass is distributed versus particle diameter. "table" => use a table to describe distribution "lognormal" => use a clipped lognormal distribution	"table"
density	1D array of particle density (kg/m^3) for aerosol releases with one value for each mass bin in the table distribution. Note if mass_distrib = "lognormal" all particles are assumed to have the same density which will be equal to the first element of this array. (Maximum array size = 100)	1000.
Parameters needed to define mass distribution using table option		
m_bin_fract	array of mass fractions for each mass bin in the table. (Maximum array size = 100) ($\sum$ m_bin_fract = 1.0) *To model a gas set m_bin_fract = 1.0 and m_bin_diam_max = m_bin_diam_min = 0.0* *Note: m_bin_fract is reinitialized to the default before reading each source_param namelist.*	1.0
m_bin_diam_max	array of maximum particle diameters in meters for each mass bin in the table. (Maximum array size = 100)	0.
m_bin_diam_min	array of minimum particle diameters in meters for each mass bin in the table. (Maximum array size = 100) *If m_bin_diam_min = m_bin_diam_max all particles in that size bin will have the same diameter ("monodispere" aerosol)*	0.
Parameters needed to define mass distribution using lognormal option		
mmd	mass median particle diameter in meters of the lognormal distribution. For radiological sources this parameter can represent the activity mean particle diameter (AMD), if emiss_rates are in activity units.	

src_param		
Variable Name	Description and possible values	Defaults
gsd	geometric standard deviation for the lognormal distribution $gsd = \frac{diam(50\%)}{diam(16\%)} = \frac{diam(84\%)}{diam(50\%)}$	
diam_max	maximum particle diameter in meters for a clipped lognormal distribution	$e^{(a+4b)}$ $a = \ell n(mmd)$ $b = \ell n(gsd)$
diam_min	minimum particle diameter in meters for a clipped lognormal distribution	$e^{(a+4b)}$ $a = \ell n(mmd)$ $b = \ell n(gsd)$
End mass distribution parameters		
nset_dep_vel	non-settling deposition velocity (m/s) i.e., not including the gravitational settling velocity. This can be represented as $1/r_T$, where r_T is the total integral resistance to deposition below a reference height.	0.0
precip_coeff	1D array of precipitation scavenging coefficients (s^{-1}) for each met_time.	0
decay_chain	Logical flag indicating whether decay chains will be constructed for this source. (This allows daughter products, generated by parent nuclides specified in “species” namelist variable, to be included in the calculation) .true. => decay chains will be constructed for this source .false. => decay chains will not be constructed for this source	.true.

src_param		
Variable Name	Description and possible values	Defaults
decay_param	Character (24) indicator of decay parameter being specified for first order decay a(t) = a_0 exp[- λ (t - t_0)]. “none” => no decay parameter specified in namelist. If decay_chain = .true., then the decay constants from that file will be used; otherwise no decay is calculated. $\lambda = 0$ “half_life” => use the half life of the substance. λ = ln{2} / half_life “efolding_t => use the efolding time. λ = 1 / efolding_t “lambda => enter λ directly Note: If there are more than one species in the source, the decay constant is applied to all species. For decay and growth of multiple species in radioactive decay chains, use a value of “none” to use the values in the decay_chains_file.	“none”
half_life	the species half life in seconds. (See decay_param)	
efolding_t	the species efolding time in seconds. (See decay_param)	
lambda	the species decay rate, λ, in inverse seconds. (See decay_param)	
dt_hold_str	Character (40) string to specify hold up time to decay and grow radioactive species before actual start of simulation. String format is “days::hours:minutes:seconds”, where days is the integer number of days, hours is the integer number of hour, minutes is an integer number of minutes, and seconds is the floating point number of seconds. Since the string is interpreted from the right leading units may be omitted, i.e. “200.5” is interpreted as 200.5 seconds, “10:5” is interpreted as 10 minutes and 5 seconds. All separators to the right must be entered, i.e. “2:0” or “2:” is interpreted as 2 minutes, “2::0:0:0” or “2::::” is interpreted as 2 days.	

src_param		
Variable Name	Description and possible values	Defaults
uv_decay	Logical flag indicating that the source will undergo decay due to UV radiation. .true. -> particles experience UV decay .false. -> no UV decay	.false.
uv_decay_min	The minimum UV decay rate (% per minute) for the source material	0
uv_decay_max	The maximum UV decay rate (% per minute) for the source material	0

Table 6. Namelist bin_param contents (lodi.nml)

bin_param		
Variable Name	Description and possible values	Defaults
bin_id	Character string (40) used to identify this bin.	
type	Character (24) to identify the type of bin "air" => an air concentration bin "dep_ dry" => a surface bin for dry deposition "dep_ wet" => a surface bin for wet deposition	
orientation	Character (8) indicator of the coordinates of an air type bin "xy" => generate "horizontal" slice at constant z or (z-z_g). (*See bin_agl_flg.*) "xsigma" => generate a constant y slice. "ysigma" => generate a constant x slice. "xysigma" => generate a full 3D field	
position	Coordinate value at which to place an air type concentration bin in sampling direction, i.e. y position if "xsigma", x position if "ysigma", and z or (z-z_g) position if "xy". (*See bin_agl_flg.*)	0
width	Sampling width in meters in the direction perpendicular to the 2D bin. (Note this is ignored for deposition bins.)	0

bin_param

Variable Name	Description and possible values	Defaults
dt_samp_str	Character (40) string indicating: 1) If samp_type = “pk_average” then dt_samp_str represents the peak averaging interval. 2) Otherwise it is the time interval over which to integrate (average) the air concentrations. dt_samp must be ≤ dt_bin_out Integration (averaging) period for the n^{th} interval is from (n*dt_bin_out - dt_samp) to n*dt_bin_out. 3) This is not used for instantaneous air bins or any deposition bins. String format is “days::hours:minutes:seconds”, where days is the integer number of days, hours is the integer number of hour, minutes is an integer number of minutes, and seconds is the floating point number of seconds. Since the string is interpreted from the right leading units may be omitted, i.e. “200.5” is interpreted as 200.5 seconds, “10:5” is interpreted as 10 minutes and 5 seconds. All separators to the right must be entered, i.e. “2:0” or “2:” is interpreted as 2 minutes, “2::0:0:0” or “2::::” is interpreted as 2 days.	
dt_bin_out_str	Character (40) string indicating the time interval between output dumps for this bin. *If samp_type = “pk_average” then the value of dt_bin_out must be an integer multiple of dt_samp, i.e., dt_bin_out = m * value of dt_samp.* String format is “days::hours:minutes:seconds”. See dt_samp.	

bin_param		
Variable Name	Description and possible values	Defaults
samp_type	Character (24) indicator of the type of concentration to be calculated. “average” => calculate the average air concentration from (output time - dt_samp) to output time “integrated” => calculate integrated air concentration or the integrated deposition exposure. For air bins this is from (output time - dt_samp) to output time “pk_average” => calculate the peak of the averaged air concentrations for consecutive dt_samp intervals that occurred between (n-1)*dt_bin_out and n*dt_bin_out. “instantaneous” => calculate the instantaneous air concentration or accumulated deposition at output time where the nth output time = n*dt_bin_out.	“integrated”
bin_agl_flg	Logical flag indicating whether the sampling height is to be interpreted as height above mean sea level (MSL) or height above ground (AGL) .true. => position is z AGL .false. => position is z MSL	.true.
source_list	1D character (40) array of source identifiers to be accumulated in the concentration calculation. (T*hese must correspond to the source_id strings listed in the source input.*) (*Maximum is 50.*) *Note: source_list is reinitialized after each bin_param namelist is read.*	

bin_param		
Variable Name	Description and possible values	Defaults
species_name	Character (40) string specifying the name of the species to be included in this bin. *Note: only one species can be included in an output bin. However, the same species from multiple sources can be combined in a single output bin (see "source_list".)*	

Table 7. Namelist turb_param contents (lodi.nml)

turb_param		
Variable Name	Descriptions and Possible Values	Default
read_adapt_turb	logical flag to determine whether to read turbulence fields from ADAPT or calculate and grid them from namelist input. .true. => read turbulence fields: K_z, σ_v^2, t_L, u_*, L^{-1}, h_{PBL}, from ADAPT met files .false. => calculate from analytic expressions and namelist values. *Note: if read_adapt_turb is true the following namelist variables dealing with turbulence specification as well as bldepth are ignored.*	.false. *Note: the NARAC system sets read_adapt_turb to .true. as the default.*
turb_param_z	character (24) string indicating the vertical turbulence parameterization of K_z: "linear_power" =>K_z is a function of z to a power "simthry" => K_z is derived via similarity theory "constantkz" => K_z is constant in vertical	"simthry"
Parameters for linear power turbulence model (turb_param_z = "linear_power")		
kz0_slope	$\partial K_z / \partial z$ at z_g for the "linear_power" parameterization of K_z (m/s)	
kz_scale_hgt	scale height factor for the "linear_power" K_z model (m)	
kz_power	power used in "linear_power" K_z model	
Parameters for similarity theory turbulence models (turb_param_z = "simthry") and/or turb_param_h = "sigmav_simthry"		
ustar	1D array of friction velocities (m/s). (One for each met_time.) *If ustar(1) is < 0 ustar will be calculated by the code for each met_time.*	-99999.0

turb_param

Variable Name	Descriptions and Possible Values	Default
z0	1D array of roughness heights in meters. (One for each grid.) *Only used to calculate ustar i.e., when ustar(1) < 0.*	
bldepth	1D array of boundary layer depths (m AGL). (One for each met_time.)	-99999.0
obulen_inv	1D array of Obukhov length inverses (m^{-1}). (One for each met_time.)	
kz_c	constant *c* used in the "simthry" K_z parameterization	4
kz_trop	value for the eddy diffusivity (K_z) in m^2/s above the boundary layer	0.01
Parameters for constant vertical turbulence model (turb_param_z = "constantkz")		
kz_const	constant value for "constant" K_z parameterization	
End parameters for vertical turbulence, K_z, models		
turb_param_h	character (24) string indicating the horizontal turbulence parametization model: "constantkh" => use a constant value for K_x and K_y "sigmav" => use constant input σ_v to calculate K_x and K_y "sigmav_simthry" => use variable σ_v calculated via similarity theory to calculate K_x and K_y	"sigmav_simthry"
Parameters for constant horizontal turbulence model (turb_param_h = "constant *kh*")		
*Kh*_const	constant value for "constant *Kh*" K_x and K_y parameterizations (m^2/s)	
Parameters for σ_v turbulence models (turb_param_h = "sigmav") and/or (turb_param_h = "sigmav_simthry") (*also requires input similarity theory parameters* - see above)		
*Kh*_d	constant *d* used in the "sigmav" and "sigmav_simthry" K_x – K_y parameterization	0.9

turb_param		
Variable Name	Descriptions and Possible Values	Default
t_lagran_h	1D array of turbulence time scale, T_i, (s) values, with one value for each met_time for the "sigmav" and "sigmav_simthry" K_x and K_y parameterizations.	if turb_param_h = sigmav, then default values is 1000 if turb_param_h = sigmav_simthry and t_lagran_h is either unfilled or assigned (indicated by a value of -99999.), then the code will calculate the value
sigma_v	1D array of σ_v (m/s) (one for each met_time) used in the "sigmav" $K_x – K_y$ parameterization or 1D array of measured σ_v (m/s) (one for each met_time) used in "sigmav_simthry" $K_x – K_y$ parameterization to scale calculated σ_v (optional, if this is input sigmav_meas_hgt must also be input)	
sigmav_meas_hgt	1D array of the heights (m AGL) of the measured values σ_v Used only in "sigmav_simthry" $K_x – K_y$ parameterization when sigma_v is input.	
sigmav_min	1D array of minimum σ_v (m/s) (one for each met_time). Used only for "sigmav_simthry" $K_x – K_y$ parameterization. Must be set to 0.0 to supress minimum σ_v.	0.5
zero_kx	Logical flag to zero K_x (x-direction diffusion) .true. => zero K_x .false.=> do not zero K_x *Note, should be used by developers only.*	.false.
zero_ky	Logical flag to zero K_y (y-direction diffusion) .true. => zero K_y .false.=> do not zero K_y *Note, should be used by developers only.*	.false.

<table>
<tr><th colspan="3">turb_param</th></tr>
<tr><th>Variable Name</th><th>Descriptions and Possible Values</th><th>Default</th></tr>
<tr><td>zero_kz</td><td>Logical flag to zero K_z (vertical diffusion)
.true. => zero K_z
.false.=> do not zero K_z
<em>Note, should be used by developers only.</em></td><td>.false.</td></tr>
</table>

Table 8. Namelist met_param contents (lodi.nml)

Variable Name	Description and possible values	Defaults
zp_top	1D array of length "num_met_times" of the upper bound for precipitation height in meters MSL below which precipitation scavenging is possible. *(See precip_coeff)*	ztop from met grid 1.

Table 9. Namelist receptor_param contents (lodi.nml)

receptor_param		
Variable Name	Description and possible values	Defaults
receptor_id	Character string (40) used to identify this moving receptor.	
rec_time_strs	1D character (40) array of valid receptor times for the moving receptor variables *(Maximum number is 50)* *Note: rec_time_strs is reinitialized after each receptor_param namelist is read.*	
num_boxes	Integer array of length 3 containing the number of sampling volumes to be defined for this receptor in the x, y, and z directions respectively.	1, 1, 1
delta_tot	Array of length 3 containing the total length of the receptor in the x, y, and z directions respectively	1.0, 1.0, 1.0
delta_s	Array of length 3 containing the length of the interior sampling volumes in the x, y, and z directions respectively	1.0, 1.0, 1.0
xcen_rec	1D array containing the x positions of the receptor at each of the times listed in “rec_time_strs”	
ycen_rec	1D array containing the y positions of the receptor at each of the times listed in “rec_time_strs”	
zcen_rec	1D array containing the z positions (either AGL or MSL see “agl_flg_zcen”) of the receptor at each of the times listed in “rec_time_strs”	
agl_flg_zcen	Logical flag indicating whether the receptor center heights is to be interpreted as height above mean sea level (MSL) or height above ground (AGL) .true. => center positions are z AGL .false. => center positions are z MSL	.true.
dt_rec_out_str	Character (40) string indicating the time interval between output dumps for this receptor. String format is “days::hours:minutes:seconds”.	

receptor_param		
Variable Name	Description and possible values	Defaults
dt_rec_samp_str	Character (40) string indicating the time interval over which to average or integrate air concentration for this receptor. String format is “days::hours:minutes:seconds”.	
rec_samp_type	Character (24) indicator of the type of concentration to be calculated. “average” => calculate the average air concentration from (output time - dt_rec_samp) to output time “integrated” => calculate integrated air concentration or the integrated deposition exposure from (output time - dt_rec_samp) to output time “pk_average” => calculate the peak of the averaged air concentrations for consecutive dt_rec_samp intervals that occurred between (n-1)*dt_rec_out and n*dt_rec_out. “instantaneous” => calculate the instantaneous air concentration or accumulated deposition at dump_time where the nth output time = n*dt_rec_out.	“integrated”
rec_source_lst	1D character (40) array of source identifiers to be accumulated in the concentration calculation. (*These must correspond to the source_id strings listed in the source input.*) *Note: rec_source_list is reinitialized after each receptor_param namelist is read.*	
species_name	Character (40) string specifying the name of the species to be included in the sampling volume.	

15.2 Namelists contained in file 'lodi_files.nml'

Table 10. Namelist grid_name contents (lodi_files.nml)

Variable Name	Description and possible values	Defaults
num_m_grids	Integer number of meteorological data grids to be used. (Legal values 1, 2, or 3)	1
m_grid_name	1D array of length "num_m_grids" of Character (160) names for meteorological data grid files	
c_grid_name	Character (160) name of the base concentration grid file	

Table 11. Namelist metfiles contents (lodi_files.nml)

Variable Name	Description and possible values	Defaults
grid_num	Integer number corresponding to the number of the grid to which this namelist applies.	
met_file_name	1D array of length "num_met_times" of Character (160) file names for the meteorological data sets on grid number "grid_num". (*Must have "num_m_grids" metfiles namelists total.*)	

Table 12. Namelist decay_chains_file contents (lodi_files.nml)

Variable Name	Description and possible values	Defaults
decay_chains_file_name	Character (160) name of the ascii file containing the decay chain constants (branching fraction).	"decaychains.dat"

Table 13. Namelist particle_file contents (lodi_files.nml)

Variable Name	Description and possible values	Defaults
particle_file_name	Character (160) name of the netCDF file from which to read particle information for sources with src_generation_method = “continuation”	“mpart<date/time>.nc”
This namelist is only required if there is a source with src_generation_method = “continuation”.		

Table 14. Namelist dep_files contents (lodi_files.nml)

Variable Name	Description and possible values	Defaults
dep_file_name	Character (160) name of the netCDF master deposition file from which to read deposition data for all species in a source with src_generation_method = “continuation”.	“mdep.nc”
This namelist is only required if there is a depositing source with src_generation_method = “continuation”.		

15.3 Note on output bin units

The units of the data for each output bin file depends on the type of bin as set by the “type” parameter in the bin namelist and the type of sampling requested as specified by the namelist value “samp_type” as well as the units of the emission rates (namelist variable “emiss_rates” in the src_param namelist) for the sources used for that bin. The src_param namelist variable “emiss_rates” may be in units of mass or radioactivity units per second with the variable “er_units_type” appropriately set to “mass” or “radioactivity”. The emission rate units when “er_units_type” is “mass” are massunit/s such as kg/s, g/s, μg/s where massunit is kg, g, and μg respectively. The emission rate units when “er_units_type” is “radioactivity” are activityunit/s such as Ci/s, Bq/s, and μCi/s where activityunit is Ci, Bq, and μCi respectively . The output units for each bin type and samp_type are as follows, where “massactivityunits” is the mass or activity units used in emission rates:

Table 15. Bin output units

Bin type “type”	Sampling type “samp_type”	Units
air	average	massactivityunits m^{-3}
air	integrated	massactivityunits sec m^{-3}
air	pk_average	massactivityunits m^{-3}
air	instantaneous	massactivityunits m^{-3}
dep_dry or dep_wet	instantaneous	massactivityunits m^{-2}
dep_dry or dep_wet	integrated	massactivityunits sec m^{-2}

Thus, for bin type = “air”, samp_type = “average” and “emiss_rates” in units of (kg s^{-1}), the bin data in the output files will be average air concentration in units of (kg m^{-3}) and for bin type= “dep_dry”, samp_type = “integrated”, and “emiss_rates” in units of (Ci s^{-1}), the bin data in the output files will be integrated dry deposition in units of (Ci s m^{-2}).

15.4 Notes on continuing a simulation

A previously completed LODI simulation may be continued by specifying the appropriate parameters in the input namelists. The following lodi.nml parameters in the old run need to be changed for a new, continuation run:

&prob_setup
    tstart_str =   new, continued run start time
    tstop_str =   new, continued run stop time

&src_param
    src_generation_method =   'continuation'

If source material is to be emitted in the continued run, the following parameters also need to be updated for each source:

&src_param
    start_time_str
    stop_time_str
    max_num_part = number of new particles to be generated during continued run (the value of max_num_part will be ignored if no new particles are going to be generated in the continued run based on the source start and stop times)
    er_time_strs
    emiss_rates

In the lodi_files.nml namelist, the pathnames for the files containing the particle information (the mpart<date/time>.nc file from the run to be continued) and deposition file (mdep.nc from the run to be continued), need to be specified:

&particle_file
    particle_file_name

&dep_file
    dep_file_name

(It is recommended that the continuation run be done in a new directory with these pathnames pointing to the files in the directory for the old run, to avoid overwriting these files with output from the new run).

16. Example Problem

The following section presents a description of a sample problem[*], some of the results from the simulation and the listing of the text input and output files from the simulation. The figures illustrating the simulation results were made via the GTX graphics package.

16.1 Problem description

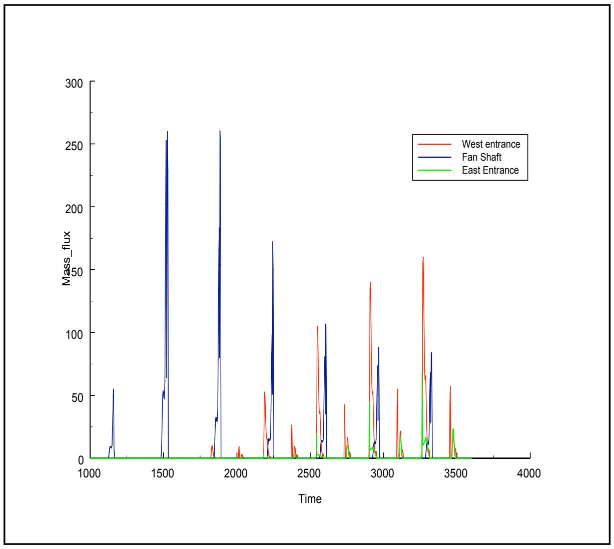

Figure 7. The emission rates as a function of time for the three different sources.

This example simulates a release within a subway station where some of the contaminant is discharged into the free atmosphere. The leaks to the outside are located at three different places: the west station entrance, a ventilation shaft, and the east station entrance. Because these locations are different distances from the release point, the contaminant reaches each at a different time. The pulsing of the flow within the station induced by the piston effects of the trains entering and leaving the station causes the emissions to be highly time dependent and distinct for each source. Figure 7 shows the emission rates used in the example simulation. From this it can be seen that west entrance begins emitting first followed by the ventilation shaft and then the east entrance. Also of note is the relative sizes of the emisssions. The west entrance emits the most and the east entrance emits an order of magnitude less contaminant.

The example simulation lasted three hours. The met grid was 30 km × 30 km × 3 km and the concentration grid was 25 km × 25 km × 3 km. Figure 8 shows the horizontal concentration grid. The fine grading around the sources and the expanding grid size in each direction is clearly seen. The sources were treated as near surface Gaussian sources. The contaminant released was treated as a gas with a small decay rate. The vertical turbulence was modeled using similarity theory. The simulation used hourly gridded wind fields (four fields were necessary) developed by ADAPT from the available observations. Four sampling bins were defined: the three hour integrated concentration from each source and the total three hour integrated concentration from all sources. The particle positions were output every half hour.

[*] This example is from an earlier version of LODI and may contain some differences from version 1.0 of LODI

16.2 Results

Figure 9 shows the instantaneous plan view of the particles at one hour, two hours, and three hours. This reflects the initial light ENE wind which increases in speed and backs to the NE and then switches to an east wind during the final hour.

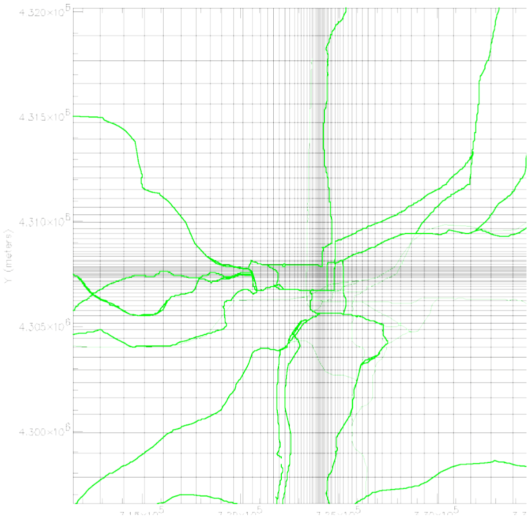

Figure 8. Concentration grid and map.

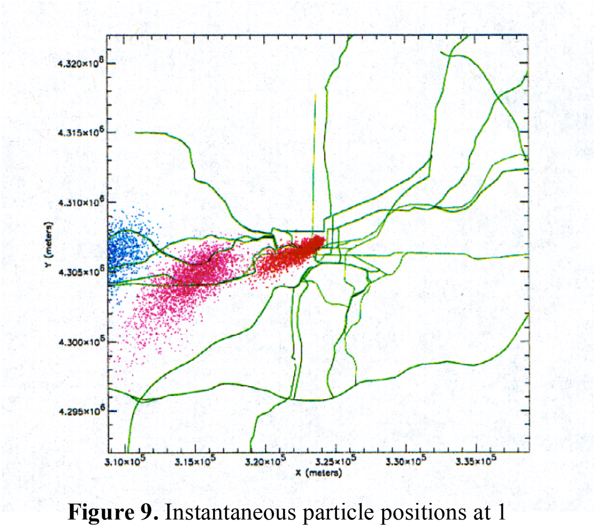

Figure 9. Instantaneous particle positions at 1 hour, 2 hours, and 3 hours.

The next three figures, Figures 10 - 12, show the plan view of the three-hour integrated, near-surface, air concentration resulting from the release at each of the three source locations individually.

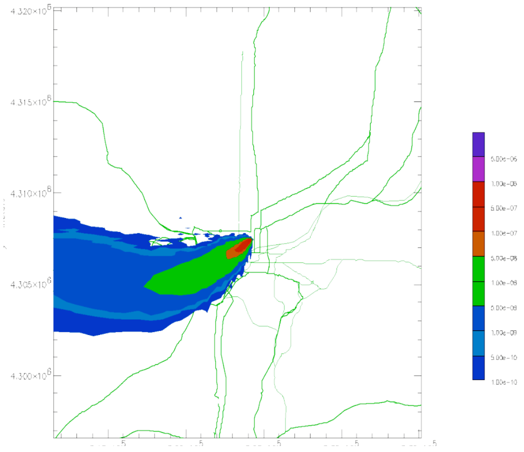

Figure 10. Three-hour integrated air concentration from the west entrance (bin 1).

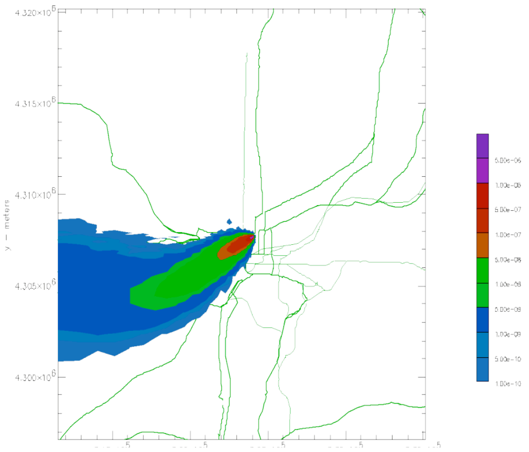

Figure 11. Three-hour integrated air concentration from the fan shaft (bin 2).

Because the third source (east entrance) was of much smaller magnitude, it contributed significantly less to the total concentration field as can be seen in the Figure 12.

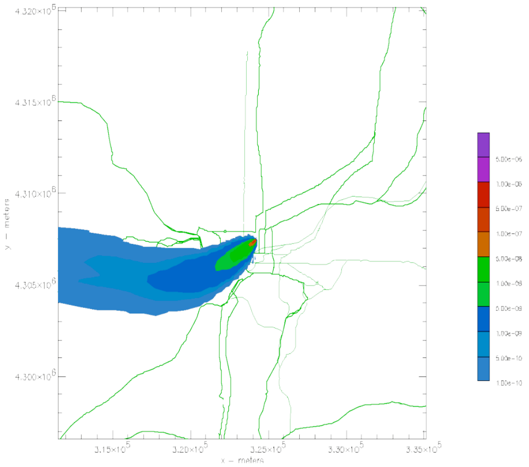

Figure 12. Three-hour integrated air concentration from east entrance (bin 3).

Finally, Figure 13 shows a plan view of the total three-hour integrated, near-surface, air concentration field resulting from the releases at all three source points. Because the sources were very close together, they are not individually evident in the total integrated concentration plot. (On a blow-up of this plot the highest concentration contour does show two distinct centers around the two larger sources.) However, the total integrated concentration field is clearly the sum of the three individual integrated concentrations. (It is in fact possible to construct this field by simply adding the three individual fields via a post processor.)

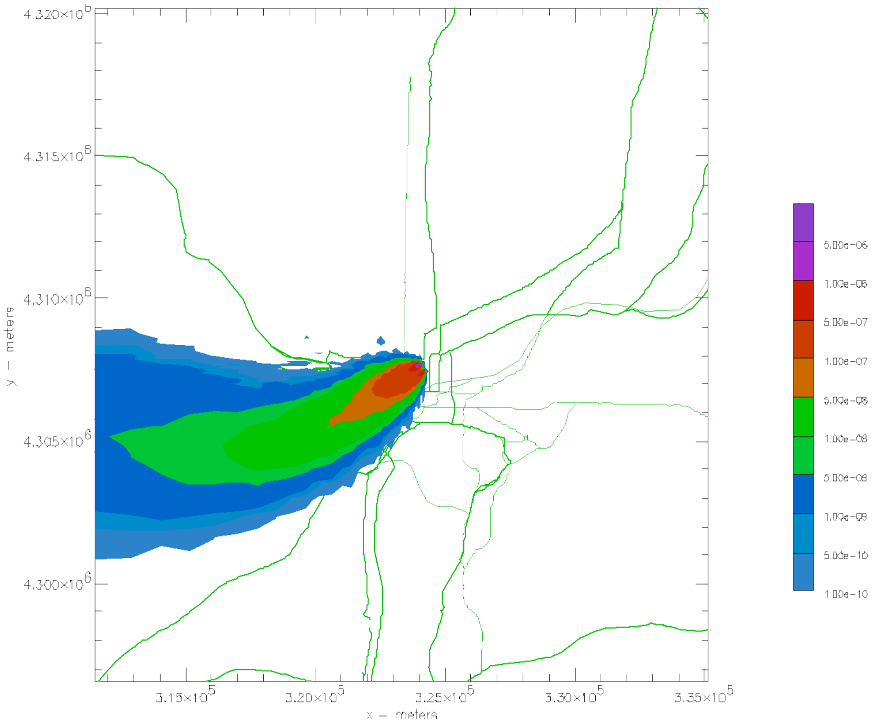

Figure 13. Three-hour integrated air concentration from all sources (bin 4).

16.3 The example lodi.nml file

```
&prob_setup
   title = 'Manual Example Simulation'
   tstart_str = '1997JUL11_210000'   tstop_str = '1997Jul12_000000'
   dt_part_out_str = '30:0.0'
   nbins = 4
   nsrc  = 3
   rdm_dist = 'gauss'
   met_format = 'arac'
   num_met_times = 4
   met_time_strs = '1997JUL11_210000' '1997JUL11_220000' '1997JUL11_230000' '1997JUL12_000000'
/
&thist_param
/
&src_param
   source_id = 'West Entrance'

   max_num_part   = 15000
   start_time_str = '1997JUL11_212400'
   stop_time_str  = '1997JUL11_215830'

   geom_type      = 2
   geom_time_strs =  '1997JUL11_210000'
   mean_x         =   324211.0
   std_x          =        1.618
   cutoff_dx_min  =        3.236
   cutoff_dx_max  =        3.236

   mean_y         =  4307433.0
   std_y          =        1.618
   cutoff_dy_min  =        3.236
   cutoff_dy_max  =        3.236

   mean_z         =  20.00
   std_z          =  10.0
   cutoff_dz_min  =  20.00
   cutoff_dz_max  =  20.0
   src_agl_flg    = .true.

   er_time_strs   = '1997JUL11_212400'  '1997JUL11_212430'
                    '1997JUL11_212500'  '1997JUL11_212530'  '1997JUL11_212700'
                    '1997JUL11_212730'  '1997JUL11_212800'  '1997JUL11_212830'
                    '1997JUL11_213000'  '1997JUL11_213030'  '1997JUL11_213100'
                    '1997JUL11_213130'  '1997JUL11_213300'  '1997JUL11_213330'
                    '1997JUL11_213400'  '1997JUL11_213430'  '1997JUL11_213600'
                    '1997JUL11_213630'  '1997JUL11_213700'  '1997JUL11_213730'
                    '1997JUL11_213900'  '1997JUL11_213930'  '1997JUL11_214000'
                    '1997JUL11_214030'  '1997JUL11_214200'  '1997JUL11_214230'
                    '1997JUL11_214300'  '1997JUL11_214330'  '1997JUL11_214500'
                    '1997JUL11_214530'  '1997JUL11_214600'  '1997JUL11_214630'
                    '1997JUL11_214800'  '1997JUL11_214830'  '1997JUL11_214900'
                    '1997JUL11_214930'  '1997JUL11_215100'  '1997JUL11_215130'
                    '1997JUL11_215200'  '1997JUL11_215230'  '1997JUL11_215400'
                    '1997JUL11_215430'  '1997JUL11_215500'  '1997JUL11_215530'
                    '1997JUL11_215700'  '1997JUL11_215730'  '1997JUL11_215800'

   emiss_rates    =  1.531357E-09        6.794410E-09
                     1.625875E-15        0.000000E+00        4.429808E-12
                     9.953041E-08        5.168532E-09        0.000000E+00
                     1.682804E-06        2.669806E-06        1.343364E-08
                     0.000000E+00        1.119667E-10        2.609287E-06
                     2.460253E-07        0.000000E+00        9.982227E-06
                     1.754632E-05        3.492722E-07        0.000000E+00
                     3.284300E-10        7.841972E-06        9.095280E-07
                     0.000000E+00        2.040497E-05        3.787553E-05
                     1.117866E-06        0.000000E+00        5.365783E-10
                     1.298812E-05        1.666261E-06        0.000000E+00
                     2.744960E-05        5.301442E-05        1.923885E-06
                     0.000000E+00        6.941883E-10        1.688177E-05
                     2.242999E-06        0.000000E+00        3.174034E-05
                     6.296690E-05        2.538894E-06        0.000000E+00
                     7.315425E-10        1.791619E-05        2.497931E-06

   species        = 'toxic agent'
   decay_param    = 'efolding_t'
   efolding_t     =  5969.9497
   mass_distrib   = 'table'
   m_bin_fract    =  1.0
   m_bin_diam_max =  0.0
   m_bin_diam_min =  0.0
   density        =  1000.
   precip_coeff   =     0.
/
&src_param
   source_id = 'Fan Shaft'

   max_num_part   = 15000
   start_time_str = '1997JUL11_211830'
   stop_time_str  = '1997JUL11_215530'

   geom_type      = 2
   geom_time_strs =  '1997JUL11_210000'
   mean_x         =   324095.0
   std_x          =        1.360
   cutoff_dx_min  =        2.719
   cutoff_dx_max  =        2.719

   mean_y         =  4307691.0
   std_y          =        1.360
   cutoff_dy_min  =        2.719
   cutoff_dy_max  =        2.719

   mean_z         =  15.0
   std_z          =   7.5
   cutoff_dz_min  =  15.0
   cutoff_dz_max  =  15.0
   src_agl_flg    = .true.

   er_time_strs   = '1997JUL11_211830'  '1997JUL11_211900'
                    '1997JUL11_211930'  '1997JUL11_212430'  '1997JUL11_212500'
                    '1997JUL11_212530'  '1997JUL11_213030'  '1997JUL11_213100'
                    '1997JUL11_213130'  '1997JUL11_213630'  '1997JUL11_213700'
                    '1997JUL11_213730'  '1997JUL11_214230'  '1997JUL11_214300'
                    '1997JUL11_214330'  '1997JUL11_214830'  '1997JUL11_214900'
                    '1997JUL11_214930'  '1997JUL11_215430'  '1997JUL11_215500'

   emiss_rates    =  3.447288E-06        1.763338E-05
                     0.000000E+00        1.960235E-05        1.465307E-04
                     0.000000E+00        1.185590E-05        1.193257E-04
                     0.000000E+00        5.571682E-06        6.619260E-05
                     0.000000E+00        5.141698E-06        5.092920E-05
                     0.000000E+00        4.685895E-06        4.393257E-05
                     0.000000E+00        4.473370E-06        4.229501E-05

   species        = 'toxic agent'
   decay_param    = 'efolding_t'
   efolding_t     =  5969.9497
   mass_distrib   = 'table'
   m_bin_fract    =  1.0
   m_bin_diam_max =  0.0
   m_bin_diam_min =  0.0
   precip_coeff   =     0.
/
&src_param
   source_id = 'East Entrance'

   max_num_part   = 15000
   start_time_str = '1997JUL11_212730'
   stop_time_str  = '1997JUL11_215830'

   geom_type      = 2
   geom_time_strs =  '1997JUL11_210000'
   mean_x         =   324211.0
   std_x          =        1.541
   cutoff_dx_min  =        3.081
   cutoff_dx_max  =        3.081

   mean_y         =  4307422.0
   std_y          =        1.541
   cutoff_dy_min  =        3.081
   cutoff_dy_max  =        3.081

   mean_z         =  17.5
   std_z          =   8.75
   cutoff_dz_min  =  17.5
   cutoff_dz_max  =  17.5
   src_agl_flg    = .true.

   er_time_strs   = '1997JUL11_212730'  '1997JUL11_212800'
                    '1997JUL11_212830'  '1997JUL11_213000'  '1997JUL11_213030'
                    '1997JUL11_213100'  '1997JUL11_213130'  '1997JUL11_213300'
                    '1997JUL11_213330'  '1997JUL11_213400'  '1997JUL11_213430'
                    '1997JUL11_213600'  '1997JUL11_213630'  '1997JUL11_213700'
                    '1997JUL11_213730'  '1997JUL11_213800'  '1997JUL11_213900'
                    '1997JUL11_213930'  '1997JUL11_214000'  '1997JUL11_214030'
                    '1997JUL11_214200'  '1997JUL11_214230'  '1997JUL11_214300'
                    '1997JUL11_214330'  '1997JUL11_214400'  '1997JUL11_214500'
                    '1997JUL11_214530'  '1997JUL11_214600'  '1997JUL11_214630'
                    '1997JUL11_214800'  '1997JUL11_214830'  '1997JUL11_214900'
                    '1997JUL11_214930'  '1997JUL11_215000'  '1997JUL11_215100'
                    '1997JUL11_215130'  '1997JUL11_215200'  '1997JUL11_215230'
                    '1997JUL11_215400'  '1997JUL11_215430'  '1997JUL11_215500'
                    '1997JUL11_215530'  '1997JUL11_215600'  '1997JUL11_215700'
                    '1997JUL11_215730'  '1997JUL11_215800'

   emiss_rates    =  2.080777E-11        3.979240E-13
                     0.000000E+00        1.965070E-09        1.953067E-10
                     6.747998E-13        0.000000E+00        6.680792E-13
                     7.974416E-08        4.009359E-09        0.000000E+00
                     4.277222E-07        1.703274E-07        7.716790E-09
                     5.476433E-13        0.000000E+00        7.458658E-12
                     1.177383E-06        1.262383E-07        0.000000E+00
                     2.785265E-06        2.292388E-06        2.288121E-07
                     1.593742E-11        0.000000E+00        2.099075E-11
                     3.696526E-06        5.633727E-07        0.000000E+00
                     6.604280E-06        7.422975E-06        9.255893E-07
                     6.424525E-11        0.000000E+00        3.467233E-11
                     6.463428E-06        1.184431E-06        0.000000E+00
                     1.013852E-05        1.332342E-05        1.832922E-06
                     1.270732E-10        0.000000E+00        4.606950E-11
                     8.810075E-06        1.751087E-06

   species        = 'toxic agent'
   decay_param    = 'efolding_t'
   efolding_t     =  5969.9497
   mass_distrib   = 'table'
   m_bin_fract    =  1.0
   m_bin_diam_max =  0.0
   m_bin_diam_min =  0.0
   precip_coeff   =     0.
/
&bin_param
   bin_id         = 'Bin 1 - 3 hr integrated air - west entrance'
   type           = 'air'
   source_list    = 'West Entrance'
   orientation    = 'xy'
   bin_agl_flg    = .true.
   position       =    5.
   width          =   10.
   dt_samp_str    = '3:0:0.0'
   dt_bin_out_str = '3:0:0.0'
   samp_type      = 'integrated'
/
&bin_param
   bin_id         = 'Bin 2 - 3 hr integrated air - fan shaft'
   type           = 'air'
   source_list    = 'Fan Shaft'
   orientation    = 'xy'
   bin_agl_flg    = .true.
   position       =    5.
   width          =   10.
   dt_samp_str    = '3:0:0.0'
   dt_bin_out_str = '3:0:0.0'
   samp_type      = 'integrated'
/
&bin_param
   bin_id         = 'Bin 3 - 3 hr integrated air - east entrance'
   type           = 'air'
   source_list    = 'East Entrance'
   orientation    = 'xy'
   bin_agl_flg    = .true.
   position       =    5.
   width          =   10.
   dt_samp_str    = '3:0:0.0'
   dt_bin_out_str = '3:0:0.0'
   samp_type      = 'integrated'
/
&bin_param
   bin_id         = 'Bin 4 - 3 hr integrated air - all sources'
   type           = 'air'
   source_list    = 'West Entrance' 'Fan Shaft' 'East Entrance'
   orientation    = 'xy'
   bin_agl_flg    = .true.
   position       =    5.
   width          =   10.
   dt_samp_str    = '3:0:0.0'
   dt_bin_out_str = '3:0:0.0'
   samp_type      = 'integrated'
/
&turb_param
   turb_param_z = 'simthry'
   z0           = 1.0
   obulen_inv   = 0.02 0.02 0.02 0.02
   turb_param_h = 'sigmav'
   t_lagran_h   = 50. 50. 50. 50.
   sigma_v      = 0.8 0.8 0.8 0.8
/
&met_param
/
```

16.4 The example lodi_files.nml file

```
&grid_name
   num_m_grids = 1
   m_grid_name = '/u/sugiyama/pub/subway/grid/main_____1_____30___323800__4307000_001_grd.nc'
   c_grid_name = '/u/jleone/runset/lodi/subway/conc_grid/conc_____1_____25___323318__4308375_001_grd.nc'
/
&metfiles
   grid_num      = 1
   met_file_name = '/u/sugiyama/pub/subway/day1997OCT07_30km/adapt_subway_1997OCT07_170000.nc'
                   '/u/sugiyama/pub/subway/day1997OCT07_30km/adapt_subway_1997OCT07_180000.nc'
                   '/u/sugiyama/pub/subway/day1997OCT07_30km/adapt_subway_1997OCT07_190000.nc'
                   '/u/sugiyama/pub/subway/day1997OCT07_30km/adapt_subway_1997OCT07_200000.nc'
/
```

16.5 The example output to standard out (screen)

```
 LODI version xxxxx
 This is a development version
 Time =   0.000000000000000E+000   Meteorological data file read:
 /u/sugiyama/pub/subway/day1997OCT07_30km/adapt_subway_1997OCT07_170000.nc


 Time =   0.000000000000000E+000   Meteorological data file read:
 /u/sugiyama/pub/subway/day1997OCT07_30km/adapt_subway_1997OCT07_180000.nc


  Start of lodi calculation. Time =   0.000000000000000E+000
  Time =    1800.00000000000      average timestep =    38.1109771616147
        Number of active particles =        5189
        Number of lost particles =           0
 Time =    3600.00000000000        Meteorological data file read:
 /u/sugiyama/pub/subway/day1997OCT07_30km/adapt_subway_1997OCT07_190000.nc


  Time =    3600.00000000000      average timestep =    57.9025537207995
        Number of active particles =       44998
        Number of lost particles =           0
  Time =    5400.00000000000      average timestep =    108.052828175022
        Number of active particles =       44998
        Number of lost particles =           0
 Time =    7200.00000000000        Meteorological data file read:
 /u/sugiyama/pub/subway/day1997OCT07_30km/adapt_subway_1997OCT07_200000.nc


  Time =    7200.00000000000      average timestep =    141.825443177651
        Number of active particles =       44909
        Number of lost particles =          89
  Time =    9000.00000000000      average timestep =    148.238867703543
        Number of active particles =       39645
        Number of lost particles =        5353
  Time =    10800.0000000000      average timestep =    136.800732758138
        Number of active particles =       13101
        Number of lost particles =       31897
 lodi run completed,  Time =    10800.0000000000
```

16.6 The example out_lodi file

```
 &PROB_SETUP
 TSTART_STR      = 1997JUL11_210000                        ,
 TSTOP_STR       = 1997Jul12_000000                        ,
 DT_LIMIT        =   3600.00000000000     ,
 DT_PART_OUT_STR = 30:0.0                                  ,
 OUT_PART_ASCII  = F,
 OUT_BIN_ASCII   = F,
 SOLVER_ID       = rk2     ,
 X_REG   = F,
 Y_REG   = F,
 RDM_DIST        = gauss   ,
 REFLECT = vertical,
 NBINS   =           4,
 NSRC    =           3,
 TITLE   = Manual Example Simulation                                         ,
 DT_FACT_ADV     =   1.00000000000000     ,
 DT_FACT_DIF     =   1.00000000000000     ,
 NUM_MET_TIMES   =           4,
 MET_TIME_STRS   = 1997JUL11_210000                        1997JUL11_220000
1997JUL11_230000
       1997JUL12_000000
 ,
 DZ_DEP  =   20.0000000000000     ,
 MET_FORMAT      = arac    ,
 RD_GRID = gridgen
 /
 &THIST_PARAM
 NPART_ALLT      =           0,
 PART_ALLT       = 200*0
 /
 &GRID_NAME
 NUM_M_GRIDS     =           1,
 M_GRID_NAME     = /u/sugiyama/pub/subway/grid/main_____1_____30___323800__4307000_001_grd.nc


 ,
 C_GRID_NAME     = /u/jleone/runset/lodi/subway/conc_grid/conc_____1_____25___323318__4308375_001_grd.nc

 /
 &SRC_PARAM
 GEOM_TYPE       =           2,
 MAX_NUM_PART    =       15000,
 GEOM_TIME_STRS  = 1997JUL11_210000                        unfilled                                unfilled
       unfilled                                unfilled                                unfilled
unfill
 ed                                unfilled                                unfilled
unfilled
                       unfilled                                unfilled                                unfilled
           unfilled                                unfilled                                unfilled
un
 filled                                unfilled                                unfilled
unfilled
                           unfilled                                unfilled
unfilled
               unfilled                                unfilled                                unfilled
   unfilled                                unfilled                                unfilled
unfilled
                               unfilled                                unfilled
unfilled
                   unfilled                                unfilled                                unfilled
       unfilled                                unfilled                                unfilled
unfill
 ed                                unfilled                                unfilled
unfilled
                       unfilled                                unfilled                                unfilled
           unfilled                                unfilled                                unfilled
un
 filled                                ,
 X1      = 50*0.000000000000000E+000  ,
 Y1      = 50*0.000000000000000E+000  ,
 Z1      = 50*0.000000000000000E+000  ,
 X2      = 50*0.000000000000000E+000  ,
 Y2      = 50*0.000000000000000E+000  ,
 Z2      = 50*0.000000000000000E+000  ,
 X_CENTER        = 50*0.000000000000000E+000  ,
 Y_CENTER        = 50*0.000000000000000E+000  ,
 Z_CENTER        = 50*0.000000000000000E+000  ,
 RADIUS  = 50*1.00000000000000        ,
 MEAN_X  =   324211.000000000     , 49*0.000000000000000E+000  ,
 MEAN_Y  =   4307433.00000000     , 49*0.000000000000000E+000  ,
 MEAN_Z  =   20.0000000000000     , 49*0.000000000000000E+000  ,
 STD_X   =   1.61800000000000     , 49*1.00000000000000        ,
 STD_Y   =   1.61800000000000     , 49*1.00000000000000        ,
 STD_Z   =   10.0000000000000     , 49*1.00000000000000        ,
 ANGLE_DEG       = 50*0.000000000000000E+000  ,
 CUTOFF_DX_MIN   =   3.23600000000000     , 49*0.000000000000000E+000  ,
 CUTOFF_DX_MAX   =   3.23600000000000     , 49*0.000000000000000E+000  ,
 CUTOFF_DY_MIN   =   3.23600000000000     , 49*0.000000000000000E+000  ,
 CUTOFF_DY_MAX   =   3.23600000000000     , 49*0.000000000000000E+000  ,
 CUTOFF_DZ_MIN   =   20.0000000000000     , 49*0.000000000000000E+000  ,
 CUTOFF_DZ_MAX   =   20.0000000000000     , 49*0.000000000000000E+000  ,
 X_PT    = 50*0.000000000000000E+000  ,
 Y_PT    = 50*0.000000000000000E+000  ,
 Z_PT    = 50*0.000000000000000E+000  ,
 ER_TIME_STRS    = 1997JUL11_212400                        1997JUL11_212430
1997JUL11_212500
```

```
       1997JUL11_212530                        1997JUL11_212700                        1997JUL11_212730
1997JU
 L11_212800                        1997JUL11_212830                        1997JUL11_213000
1997JUL11_213030
                       1997JUL11_213100                        1997JUL11_213130
1997JUL11_213300
           1997JUL11_213330                        1997JUL11_213400                        1997JUL11_213430
19
 97JUL11_213600                        1997JUL11_213630                        1997JUL11_213700
1997JUL11_2137
 30                        1997JUL11_213900                        1997JUL11_213930
1997JUL11_214000
               1997JUL11_214030                        1997JUL11_214200                        1997JUL11_214230
   1997JUL11_214300                        1997JUL11_214330                        1997JUL11_214500
1997JUL11_
 214530                        1997JUL11_214600                        1997JUL11_214630
1997JUL11_214800
                   1997JUL11_214830                        1997JUL11_214900
1997JUL11_214930
       1997JUL11_215100                        1997JUL11_215130                        1997JUL11_215200
1997JU
 L11_215230                        1997JUL11_215400                        1997JUL11_215430
1997JUL11_215500
                       1997JUL11_215530                        1997JUL11_215700
1997JUL11_215730
           1997JUL11_215800                        unfilled                                unfilled
un
 filled                                ,
 EMISS_RATES     =  1.531357000000000E-009,  6.794410000000000E-009,  1.625875000000000E-015,
0.000000000000000E+000,
   4.429808000000000E-012,  9.953041000000000E-008,  5.168532000000000E-009,  0.000000000000000E+000,
1.682804000000000E-006,
   2.669806000000000E-006,  1.343364000000000E-008,  0.000000000000000E+000,  1.119667000000000E-010,
2.609287000000000E-006,
   2.460253000000000E-007,  0.000000000000000E+000,  9.982227000000000E-006,  1.754632000000000E-005,
3.492722000000000E-007,
   0.000000000000000E+000,  3.284300000000000E-010,  7.841972000000001E-006,  9.095280000000000E-007,
0.000000000000000E+000,
   2.040497000000000E-005,  3.787553000000000E-005,  1.117866000000000E-006,  0.000000000000000E+000,
5.365783000000000E-010,
   1.298812000000000E-005,  1.666261000000000E-006,  0.000000000000000E+000,  2.744960000000000E-005,
5.301442000000000E-005,
   1.923885000000000E-006,  0.000000000000000E+000,  6.941883000000000E-010,  1.688177000000000E-005,
2.242999000000000E-006,
   0.000000000000000E+000,  3.174034000000000E-005,  6.296690000000000E-005,  2.538894000000000E-006,
0.000000000000000E+000,
   7.315425000000000E-010,  1.791619000000000E-005,  2.497931000000000E-006, 3*0.000000000000000E+000  ,
 SPECIES = toxic agent                                ,
 SRC_AGL_FLG     = T,
 START_TIME_STR  = 1997JUL11_212400                           ,
 STOP_TIME_STR   = 1997JUL11_215830                           ,
 DECAY_PARAM     = efolding_t                 ,
 HALF_LIFE       =  0.000000000000000E+000,
 EFOLDING_T      =   5969.94970000000     ,
 LAMBDA  =  0.000000000000000E+000,
 SOURCE_ID       = West Entrance                              ,
 DENSITY =   1000.00000000000     ,
 NSET_DEP_VEL    =  0.000000000000000E+000,
 PRECIP_COEFF    = 200*0.000000000000000E+000  ,
 MASS_DISTRIB    = table                      ,
 M_BIN_FRACT     =   1.00000000000000     , 99*-1.00000000000000       ,
 M_BIN_DIAM_MAX  = 100*0.000000000000000E+000  ,
 M_BIN_DIAM_MIN  = 100*0.000000000000000E+000  ,
 MMD     =  -1.00000000000000     ,
 GSD     =  -1.00000000000000     ,
 DIAM_MAX        =  -1.00000000000000     ,
 DIAM_MIN        =  -1.00000000000000     ,
 BUOYANCY_MODEL  = neutral                    ,
 FUEL_TYPE       = ,
 FUEL_AMT        =  0.000000000000000E+000
 /
    sum mass fraction =    1.00000000000000

 Source=            1  final mass distribution:
    mass distribution type = table
    diameter min. =   0.000000000000000E+000
    diameter max. =   0.000000000000000E+000
    mass fraction =    1.00000000000000
    total mass to be emitted =   1.011575348958701E-002
 &SRC_PARAM
 GEOM_TYPE       =           2,
 MAX_NUM_PART    =       15000,
 GEOM_TIME_STRS  = 1997JUL11_210000                        unfilled                                unfilled
       unfilled                                unfilled                                unfilled
unfill
 ed                                unfilled                                unfilled
unfilled
                       unfilled                                unfilled                                unfilled
           unfilled                                unfilled                                unfilled
un
 filled                                unfilled                                unfilled
unfilled
                           unfilled                                unfilled
unfilled
               unfilled                                unfilled                                unfilled
   unfilled                                unfilled                                unfilled
unfilled
                               unfilled                                unfilled
unfilled
                   unfilled                                unfilled                                unfilled
       unfilled                                unfilled                                unfilled
unfill
 ed                                unfilled                                unfilled
unfilled
                       unfilled                                unfilled                                unfilled
           unfilled                                unfilled                                unfilled
un
 filled                                ,
 X1      = 50*0.000000000000000E+000  ,
 Y1      = 50*0.000000000000000E+000  ,
 Z1      = 50*0.000000000000000E+000  ,
 X2      = 50*0.000000000000000E+000  ,
 Y2      = 50*0.000000000000000E+000  ,
 Z2      = 50*0.000000000000000E+000  ,
 X_CENTER        = 50*0.000000000000000E+000  ,
 Y_CENTER        = 50*0.000000000000000E+000  ,
 Z_CENTER        = 50*0.000000000000000E+000  ,
 RADIUS  = 50*1.00000000000000        ,
 MEAN_X  =   324095.000000000     , 49*0.000000000000000E+000  ,
 MEAN_Y  =   4307691.00000000     , 49*0.000000000000000E+000  ,
 MEAN_Z  =   15.0000000000000     , 49*0.000000000000000E+000  ,
 STD_X   =   1.36000000000000     , 49*1.00000000000000        ,
 STD_Y   =   1.36000000000000     , 49*1.00000000000000        ,
 STD_Z   =   7.50000000000000     , 49*1.00000000000000        ,
 ANGLE_DEG       = 50*0.000000000000000E+000  ,
 CUTOFF_DX_MIN   =   2.71900000000000     , 49*0.000000000000000E+000  ,
 CUTOFF_DX_MAX   =   2.71900000000000     , 49*0.000000000000000E+000  ,
 CUTOFF_DY_MIN   =   2.71900000000000     , 49*0.000000000000000E+000  ,
 CUTOFF_DY_MAX   =   2.71900000000000     , 49*0.000000000000000E+000  ,
 CUTOFF_DZ_MIN   =   15.0000000000000     , 49*0.000000000000000E+000  ,
 CUTOFF_DZ_MAX   =   15.0000000000000     , 49*0.000000000000000E+000  ,
 X_PT    = 50*0.000000000000000E+000  ,
 Y_PT    = 50*0.000000000000000E+000  ,
 Z_PT    = 50*0.000000000000000E+000  ,
 ER_TIME_STRS    = 1997JUL11_211830                        1997JUL11_211900
1997JUL11_211930
       1997JUL11_212430                        1997JUL11_212500                        1997JUL11_212530
1997JU
 L11_213030                        1997JUL11_213100                        1997JUL11_213130
1997JUL11_213630
                       1997JUL11_213700                        1997JUL11_213730
1997JUL11_214230
           1997JUL11_214300                        1997JUL11_214330                        1997JUL11_214830
19
 97JUL11_214900                        1997JUL11_214930                        1997JUL11_215430
1997JUL11_2155
 00                        unfilled                                unfilled
unfilled
               unfilled                                unfilled                                unfilled
   unfilled                                unfilled                                unfilled
unfilled
                               unfilled                                unfilled
unfilled
                   unfilled                                unfilled                                unfilled
       unfilled                                unfilled                                unfilled
unfill
 ed                                unfilled                                unfilled
unfilled
                       unfilled                                unfilled                                unfilled
           unfilled                                unfilled                                unfilled
un
 filled                                ,
 EMISS_RATES     =  3.447288000000000E-006,  1.763338000000000E-005,  0.000000000000000E+000,
1.960235000000000E-005,
   1.465307000000000E-004,  0.000000000000000E+000,  1.185590000000000E-005,  1.193257000000000E-004,
0.000000000000000E+000,
   5.571682000000000E-006,  6.619259999999999E-005,  0.000000000000000E+000,  5.141698000000000E-006,
5.092920000000000E-005,
   0.000000000000000E+000,  4.685895000000000E-006,  4.393257000000000E-005,  0.000000000000000E+000,
4.473370000000000E-006,
   4.229501000000000E-005,  3.284300000000000E-010,  7.841972000000001E-006,  9.095280000000000E-007,
0.000000000000000E+000,
   2.040497000000000E-005,  3.787553000000000E-005,  1.117866000000000E-006,  0.000000000000000E+000,
5.365783000000000E-010,
   1.298812000000000E-005,  1.666261000000000E-006,  0.000000000000000E+000,  2.744960000000000E-005,
5.301442000000000E-005,
   1.923885000000000E-006,  0.000000000000000E+000,  6.941883000000000E-010,  1.688177000000000E-005,
2.242999000000000E-006,
   0.000000000000000E+000,  3.174034000000000E-005,  6.296690000000000E-005,  2.538894000000000E-006,
0.000000000000000E+000,
   7.315425000000000E-010,  1.791619000000000E-005,  2.497931000000000E-006, 3*0.000000000000000E+000  ,
 SPECIES = toxic agent                             ,
 SRC_AGL_FLG     = T,
 START_TIME_STR  = 1997JUL11_211830                        ,
 STOP_TIME_STR   = 1997JUL11_215530                        ,
 DECAY_PARAM     = efolding_t              ,
 HALF_LIFE       =  0.000000000000000E+000,
 EFOLDING_T      =   5969.94970000000     ,
 LAMBDA  =  0.000000000000000E+000,
 SOURCE_ID       = Fan Shaft                          ,
 DENSITY =   1000.00000000000     ,
 NSET_DEP_VEL    =  0.000000000000000E+000,
 PRECIP_COEFF    = 200*0.000000000000000E+000  ,
 MASS_DISTRIB    = table                    ,
 M_BIN_FRACT     =   1.00000000000000     , 99*-1.00000000000000       ,
 M_BIN_DIAM_MAX  = 100*0.000000000000000E+000  ,
 M_BIN_DIAM_MIN  = 100*0.000000000000000E+000  ,
 MMD     =  -1.00000000000000     ,
 GSD     =  -1.00000000000000     ,
 DIAM_MAX        =  -1.00000000000000     ,
 DIAM_MIN        =  -1.00000000000000     ,
 BUOYANCY_MODEL  = neutral                 ,
 FUEL_TYPE       = ,
 FUEL_AMT        =  0.000000000000000E+000
 /
    sum mass fraction =    1.00000000000000

 Source=            2  final mass distribution:
    mass distribution type = table
    diameter min. =   0.000000000000000E+000
    diameter max. =   0.000000000000000E+000
    mass fraction =    1.00000000000000
    total mass to be emitted =   1.624852029000000E-002
 &SRC_PARAM
 GEOM_TYPE       =           2,
 MAX_NUM_PART    =       15000,
 GEOM_TIME_STRS  = 1997JUL11_210000                        unfilled                                unfilled
       unfilled                                unfilled                                unfilled
unfill
 ed                                unfilled                                unfilled
unfilled
                       unfilled                                unfilled                                unfilled
           unfilled                                unfilled                                unfilled
un
 filled                                unfilled                                unfilled
unfilled
                           unfilled                                unfilled
unfilled
               unfilled                                unfilled                                unfilled
   unfilled                                unfilled                                unfilled
unfilled
                               unfilled                                unfilled
unfilled
                   unfilled                                unfilled                                unfilled
       unfilled                                unfilled                                unfilled
unfill
 ed                                unfilled                                unfilled
unfilled
                       unfilled                                unfilled                                unfilled
           unfilled                                unfilled                                unfilled
un
 filled                                ,
 X1      = 50*0.000000000000000E+000  ,
 Y1      = 50*0.000000000000000E+000  ,
 Z1      = 50*0.000000000000000E+000  ,
 X2      = 50*0.000000000000000E+000  ,
 Y2      = 50*0.000000000000000E+000  ,
 Z2      = 50*0.000000000000000E+000  ,
 X_CENTER        = 50*0.000000000000000E+000  ,
 Y_CENTER        = 50*0.000000000000000E+000  ,
 Z_CENTER        = 50*0.000000000000000E+000  ,
 RADIUS  = 50*1.00000000000000        ,
 MEAN_X  =   324211.000000000     , 49*0.000000000000000E+000  ,
 MEAN_Y  =   4307422.00000000     , 49*0.000000000000000E+000  ,
 MEAN_Z  =   17.5000000000000     , 49*0.000000000000000E+000  ,
 STD_X   =   1.54100000000000     , 49*1.00000000000000        ,
 STD_Y   =   1.54100000000000     , 49*1.00000000000000        ,
 STD_Z   =   8.75000000000000     , 49*1.00000000000000        ,
 ANGLE_DEG       = 50*0.000000000000000E+000  ,
 CUTOFF_DX_MIN   =   3.08100000000000     , 49*0.000000000000000E+000  ,
 CUTOFF_DX_MAX   =   3.08100000000000     , 49*0.000000000000000E+000  ,
 CUTOFF_DY_MIN   =   3.08100000000000     , 49*0.000000000000000E+000  ,
 CUTOFF_DY_MAX   =   3.08100000000000     , 49*0.000000000000000E+000  ,
 CUTOFF_DZ_MIN   =   17.5000000000000     , 49*0.000000000000000E+000  ,
 CUTOFF_DZ_MAX   =   17.5000000000000     , 49*0.000000000000000E+000  ,
 X_PT    = 50*0.000000000000000E+000  ,
 Y_PT    = 50*0.000000000000000E+000  ,
 Z_PT    = 50*0.000000000000000E+000  ,
 ER_TIME_STRS    = 1997JUL11_212730                        1997JUL11_212800
1997JUL11_212830
       1997JUL11_213000                        1997JUL11_213030                        1997JUL11_213100
1997JU
 L11_213130                        1997JUL11_213300                        1997JUL11_213330
1997JUL11_213400
                       1997JUL11_213430                        1997JUL11_213600
1997JUL11_213630
           1997JUL11_213700                        1997JUL11_213730                        1997JUL11_213800
19
 97JUL11_213900                        1997JUL11_213930                        1997JUL11_214000
1997JUL11_2140
 30                        1997JUL11_214200                        1997JUL11_214230
1997JUL11_214300
               1997JUL11_214330                        1997JUL11_214400                        1997JUL11_214500
   1997JUL11_214530                        1997JUL11_214600                        1997JUL11_214630
1997JUL11_
 214800                        1997JUL11_214830                        1997JUL11_214900
1997JUL11_214930
                   1997JUL11_215000                        1997JUL11_215100
1997JUL11_215130
       1997JUL11_215200                        1997JUL11_215230                        1997JUL11_215400
1997JU
 L11_215430                        1997JUL11_215500                        1997JUL11_215530
1997JUL11_215600
                       1997JUL11_215700                        1997JUL11_215730
1997JUL11_215800
           unfilled                                unfilled                                unfilled
un
 filled                                ,
 EMISS_RATES     =  2.080777000000000E-011,  3.979240000000000E-013,  0.000000000000000E+000,
1.965070000000000E-009,
   1.953067000000000E-010,  6.747998000000000E-013,  0.000000000000000E+000,  6.680792000000000E-013,
7.974416000000000E-008,
   4.009359000000000E-009,  0.000000000000000E+000,  4.277222000000000E-007,  1.703274000000000E-007,
7.716790000000000E-009,
   5.476433000000000E-013,  0.000000000000000E+000,  7.458658000000000E-012,  1.177383000000000E-006,
1.262383000000000E-007,
   0.000000000000000E+000,  2.785265000000000E-006,  2.292388000000000E-006,  2.288121000000000E-007,
1.593742000000000E-011,
   0.000000000000000E+000,  2.099075000000000E-011,  3.696526000000000E-006,  5.633727000000000E-007,
0.000000000000000E+000,
   6.604280000000000E-006,  7.422975000000000E-006,  9.255893000000000E-007,  6.424525000000000E-011,
0.000000000000000E+000,
   3.467233000000000E-011,  6.463428000000000E-006,  1.184431000000000E-006,  0.000000000000000E+000,
1.013852000000000E-005,
   1.332342000000000E-005,  1.832922000000000E-006,  1.270732000000000E-010,  0.000000000000000E+000,
4.606950000000000E-011,
   8.810075000000001E-006,  1.751087000000000E-006,  2.497931000000000E-006, 3*0.000000000000000E+000  ,
 SPECIES = toxic agent                                 ,
 SRC_AGL_FLG     = T,
 START_TIME_STR  = 1997JUL11_212730                        ,
 STOP_TIME_STR   = 1997JUL11_215830                        ,
 DECAY_PARAM     = efolding_t               ,
 HALF_LIFE       =  0.000000000000000E+000,
 EFOLDING_T      =   5969.94970000000     ,
 LAMBDA  =  0.000000000000000E+000,
 SOURCE_ID       = East Entrance                           ,
 DENSITY =   1000.00000000000     ,
 NSET_DEP_VEL    =  0.000000000000000E+000,
 PRECIP_COEFF    = 200*0.000000000000000E+000  ,
 MASS_DISTRIB    = table                   ,
 M_BIN_FRACT     =   1.00000000000000     , 99*-1.00000000000000       ,
 M_BIN_DIAM_MAX  = 100*0.000000000000000E+000  ,
 M_BIN_DIAM_MIN  = 100*0.000000000000000E+000  ,
 MMD     =  -1.00000000000000     ,
 GSD     =  -1.00000000000000     ,
 DIAM_MAX        =  -1.00000000000000     ,
 DIAM_MIN        =  -1.00000000000000     ,
 BUOYANCY_MODEL  = neutral                 ,
 FUEL_TYPE       = ,
 FUEL_AMT        =  0.000000000000000E+000
 /
    sum mass fraction =    1.00000000000000

 Source=            3  final mass distribution:
    mass distribution type = table
    diameter min. =   0.000000000000000E+000
    diameter max. =   0.000000000000000E+000
    mass fraction =    1.00000000000000
    total mass to be emitted =   2.100561966870729E-003
 &BIN_PARAM
 ORIENTATION     = xy      ,
 POSITION        =   5.00000000000000     ,
 WIDTH   =   10.0000000000000     ,
 DT_SAMP_STR     = 3:0:0.0                         ,
 DT_BIN_OUT_STR  = 3:0:0.0                         ,
 SAMP_TYPE       = integrated              ,
 BIN_AGL_FLG     = T,
 NUM_SOURCES     =           1,
 SOURCE_LIST     = West Entrance



 ,
 BIN_ID  = Bin 1 - 3 hr integrated air - west entra,
 TYPE    = air
 /
 &BIN_PARAM
 ORIENTATION     = xy      ,
 POSITION        =   5.00000000000000     ,
 WIDTH   =   10.0000000000000     ,
 DT_SAMP_STR     = 3:0:0.0                         ,
 DT_BIN_OUT_STR  = 3:0:0.0                         ,
 SAMP_TYPE       = integrated              ,
 BIN_AGL_FLG     = T,
 NUM_SOURCES     =           1,
 SOURCE_LIST     = Fan Shaft



 ,
 BIN_ID  = Bin 2 - 3 hr integrated air - fan shaft ,
 TYPE    = air
 /
```

```
 &BIN_PARAM
 ORIENTATION     = xy      ,
 POSITION        =   5.00000000000000     ,
 WIDTH   =   10.0000000000000     ,
 DT_SAMP_STR     = 3:0:0.0                                 ,
 DT_BIN_OUT_STR  = 3:0:0.0                                 ,
 SAMP_TYPE       = integrated              ,
 BIN_AGL_FLG     = T,
 NUM_SOURCES     =           1,
 SOURCE_LIST     = East Entrance














 ,
 BIN_ID  = Bin 3 - 3 hr integrated air - east entra,
 TYPE    = air
 /
 &BIN_PARAM
 ORIENTATION     = xy      ,
 POSITION        =   5.00000000000000     ,
 WIDTH   =   10.0000000000000     ,
 DT_SAMP_STR     = 3:0:0.0                                 ,
 DT_BIN_OUT_STR  = 3:0:0.0                                 ,
 SAMP_TYPE       = integrated              ,
 BIN_AGL_FLG     = T,
 NUM_SOURCES     =           3,
 SOURCE_LIST     = West Entrance                           Fan Shaft                           East Entrance














 ,
 BIN_ID  = Bin 4 - 3 hr integrated air - all source,
 TYPE    = air
 /
 &TURB_PARAM
 TURB_PARAM_Z    = simthry                 ,
 TURB_PARAM_H    = sigmav                  ,
 KZ0_SLOPE       =  0.000000000000000E+000,
 KZ_SCALE_HGT    =  0.000000000000000E+000,
 KZ_POWER        =  0.000000000000000E+000,
 KZ_CONST        =  0.000000000000000E+000,
 KZ_C    =   4.00000000000000     ,
 KH_CONST        =  0.000000000000000E+000,
 KH_D    =  0.360000000000000     ,
 USTAR   = 200*-999999.000000000       ,
 BLDEPTH = 200*-999999.000000000       ,
 OBULEN_INV      = 4*2.000000000000000E-002  , 196*-999999.000000000       ,
 T_LAGRAN_H      = 200*50.0000000000000        ,
 SIGMA_V = 4*0.800000000000000       , 196*-999999.000000000       ,
 READ_K  = F,
 Z0      =   1.00000000000000     , 2*0.000000000000000E+000  ,
 KZ_TROP =  1.000000000000000E-002
 /
Manual Example Simulation


 current number of particles=       15000
 sum of initial masses =   1.011575348958872E-002
 fraction of mass emitted    1.00000000000017
 current number of particles=       14999
 sum of initial masses =   1.624743705531550E-002
 fraction of mass emitted   0.999933333333426
 current number of particles=       14999
 sum of initial masses =   2.100421929406012E-003
 fraction of mass emitted   0.999933333333210
```

16.7 The example lodi_con_graph.log file

```
Bin 1 - 3 hr integrated             10800.00  conc001.nc
Bin 2 - 3 hr integrated             10800.00  conc002.nc
Bin 3 - 3 hr integrated             10800.00  conc003.nc
Bin 4 - 3 hr integrated             10800.00  conc004.nc
```

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Appendix A. Turbulence Nomenclature

Symbol	Definition
h	mixed layer height (m)
k	von Karman constant (= 0.4)
K_x	along-wind eddy diffusivity (m^2/s)
K_y	cross-wind eddy diffusivity (m^2/s)
K_z	vertical eddy diffusivity (m^2/s)
K_H	horizontal eddy diffusivity (m^2/s) (Note: It is assumed that K_H =K_x=K_y)
L	Obukhov length (m)
t	time (s)
t_0	time material released into atmosphere (s).
t_a	age of material, i.e., time since released into atmosphere (s), $t_a = t – t_0$
$\bar{u}$	mean wind speed (m/s)
u_*	friction velocity (m/s)
x	downwind travel distance (m)
y	crosswind distance (m)
z	height above ground level (m)
φ_h	non-dimensional surface-layer temperature gradient function
σ_y	crosswind standard deviation of spatial distribution of concentration (m)
σ_v	standard deviation of cross-wind velocity component (m/s)
σ_w	standard deviation of vertical wind velocity component (m/s)